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Article

Major Depressive Disorder and Oxidative Stress: In Silico Investigation of Fluoxetine Activity against ROS

Cecilia Muraro [1], Marco Dalla Tiezza [1], Chiara Pavan [2], Giovanni Ribaudo [3], Giuseppe Zagotto [4] and Laura Orian [1,*]

[1] Department of Chemical Sciences University of Padova, Via Marzolo, 1-35131 Padova, Italy;
[2] Department of Medicine University of Padova, Via Giustiniani, 2-35128 Padova, Italy;
[3] Department of Molecular and Translational Medicine University of Brescia, Viale Europa, 11-25123 Brescia, Italy;
[4] Department of Pharmacological Sciences University of Padova, Via Marzolo, 5-35131 Padova, Italy;
* Correspondence: laura.orian@unipd.it; Tel.: +39-049-8275140

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	$\Delta G°_{gas}$					$\Delta G°_{water}$					$\Delta G°_{benzene}$				
Site	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$
1	-6.14	25.46	8.36	27.05	24.16	-8.46	24.00	6.62	25.26	21.71	-6.46	25.58	8.61	27.45	24.11
2	-4.81	26.79	9.70	28.38	25.49	-7.06	25.40	8.02	26.66	23.11	-5.12	26.92	9.95	28.79	25.45
4	-4.70	26.89	9.80	28.48	25.60	-6.90	25.56	8.19	26.83	23.28	-5.00	27.05	10.07	28.91	25.57
5	-3.40	28.20	11.10	29.79	26.90	-5.72	26.74	9.36	28.01	24.46	-3.73	28.32	11.34	30.19	26.85
7	-26.06	5.53	-11.56	7.12	4.23	-29.44	3.02	-14.36	4.29	0.74	-26.76	5.29	-11.69	7.15	3.81
9	-5.74	25.85	8.76	27.44	24.55	-8.83	23.63	6.26	24.90	21.35	-6.38	25.66	8.69	27.53	24.19
10	-5.91	25.69	8.59	27.28	24.39	-8.52	23.94	6.57	25.21	21.66	-6.35	25.69	8.72	27.56	24.22
11	-5.97	25.62	8.53	27.21	24.32	-8.49	23.97	6.59	25.23	21.68	-6.40	25.65	8.67	27.51	24.18
12	-6.04	25.55	8.46	27.14	24.26	-8.47	23.99	6.61	25.26	21.71	-6.44	25.61	8.63	27.47	24.14
13	-5.68	25.91	8.82	27.51	24.62	-8.90	23.56	6.19	24.83	21.28	-6.20	25.84	8.87	27.71	24.37
14	-18.31	13.28	-3.81	14.87	11.98	-21.06	11.40	-5.97	12.67	9.12	-18.88	13.16	-3.82	15.03	11.69
15	-26.88	4.71	-12.38	6.30	3.42	-30.06	2.40	-14.98	3.67	0.11	-27.89	4.15	-12.82	6.02	2.68
16	-24.24	7.36	-9.73	8.95	6.06	-31.41	1.05	-16.32	2.32	-1.23	-25.05	7.00	-9.98	8.86	5.53
17	-24.87	6.73	-10.36	8.32	5.43	-27.60	4.86	-12.52	6.13	2.57	-25.49	6.55	-10.43	8.42	5.08

Table S2. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO$^{\bullet}$, HOO$^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and CH_2=$CHOO^{\bullet}$ radicals through HAT from fluoxetine metabolites **M1** and **M2.**

M1

	$\Delta G°_{gas}$					$\Delta G°_{water}$					$\Delta G°_{benzene}$				
Site	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$
1	-3.58	28.01	10.92	29.60	26.72	-5.99	26.47	9.09	27.74	24.19	-3.92	28.12	11.15	29.99	26.65
2	-4.74	26.85	9.76	28.44	25.55	-6.94	25.52	8.15	26.79	23.24	-5.03	27.02	10.04	28.88	25.55
4	-4.99	26.60	9.51	28.19	25.31	-7.21	25.25	7.87	26.52	22.96	-5.30	26.75	9.77	28.61	25.28
5	-6.70	24.90	7.81	26.49	23.60	-8.81	23.65	6.28	24.92	21.37	-7.00	25.04	8.06	26.91	23.57
7	-30.94	0.66	-16.43	2.25	-0.64	-32.61	-0.15	-17.53	1.12	-2.44	-31.48	0.57	-16.41	2.43	-0.90
9	-5.82	25.78	8.68	27.37	24.48	-9.02	23.43	6.06	24.70	21.15	-6.47	25.57	8.60	27.44	24.10
10	-6.17	25.43	8.33	27.02	24.13	-8.81	23.65	6.27	24.92	21.36	-6.60	25.45	8.47	27.31	23.97
11	-5.88	25.71	8.62	27.30	24.41	-8.52	23.94	6.56	25.21	21.65	-6.33	25.71	8.74	27.58	24.24
12	-6.21	25.38	8.29	26.97	24.09	-8.78	23.68	6.30	24.95	21.39	-6.64	25.40	8.43	27.27	23.93
13	-6.74	24.85	7.76	26.44	23.56	-8.78	23.68	6.30	24.95	21.40	-7.09	24.95	7.98	26.82	23.48
14	-18.87	12.72	-4.37	14.31	11.42	-21.73	10.73	-6.65	12.00	8.44	-19.44	12.60	-4.38	14.47	11.13
15	-27.63	3.96	-13.13	5.55	2.67	-27.35	5.11	-12.27	6.38	2.82	-28.00	4.05	-12.93	5.91	2.58
16	-17.39	14.20	-2.89	15.80	12.91	-22.88	9.58	-7.79	10.85	7.30	-17.87	14.18	-2.80	16.05	12.71

M2

	$\Delta G°_{gas}$					$\Delta G°_{water}$					$\Delta G°_{benzene}$				
Site	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO^{\bullet}$
1	-3.16	28.44	11.34	30.03	27.14	-5.79	26.67	9.29	27.94	24.38	-3.54	28.50	11.52	30.37	27.03
5	-4.82	26.78	9.68	28.37	25.48	-5.96	26.50	9.12	27.77	24.21	-4.73	27.32	10.34	29.15	25.85
2	-4.78	26.82	9.73	28.41	25.52	-7.31	25.15	7.78	26.42	22.87	-5.14	26.9	9.92	28.77	25.43
4	-4.79	26.81	9.72	28.40	25.51	-7.09	25.37	8.00	26.64	23.09	-5.06	26.99	10.01	28.86	25.52
6a	-25.74	5.85	-11.24	7.44	4.56	-27.09	5.37	-12.00	6.64	3.09	-26.47	5.57	-11.40	7.44	4.10

Table S3. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO•, HOO•, CH_3O•, CH_3OO• and CH_2=CHOO• radicals through HAT from serotonin (2).

	$\Delta G°_{gas}$					$\Delta G°_{water}$					$\Delta G°_{benzene}$				
Site	HO•	HOO•	CH_3O•	CH_3OO•	CH_2CHOO•	HO•	HOO•	CH_3O•	CH_3OO•	CH_2CHOO•	HO•	HOO•	CH_3O•	CH_3OO•	CH_2CHOO•
1	-0.32	31.27	14.18	32.87	29.98	-2.25	30.21	12.84	31.48	27.93	-0.73	31.31	14.34	33.18	29.84
4	-5.51	26.09	9.00	27.68	24.40	-7.78	24.68	7.31	25.95	22.40	-5.80	26.24	9.27	28.11	24.77
6	-3.45	28.14	11.05	29.73	26.85	-7.31	25.15	7.77	26.42	22.87	-4.19	27.85	10.87	29.72	26.38
7	-5.05	26.55	9.46	28.14	25.25	-7.87	24.59	7.21	25.86	22.30	-5.44	26.60	9.63	28.47	25.13
9	-25.91	5.68	-11.41	7.28	4.39	-31.84	0.62	-16.75	1.89	-1.66	-26.50	5.55	-11.43	7.41	4.08
10	-28.98	2.61	-14.48	4.20	1.32	-33.41	-0.95	-18.33	0.32	-3.24	-30.02	2.02	-14.95	3.89	0.55
11	-27.30	4.30	-12.79	5.89	3.00	-27.89	4.57	-12.81	5.84	2.29	-27.48	4.56	-12.42	6.43	3.09
12	-18.02	13.58	-3.51	15.17	12.28	-23.50	8.96	-8.42	10.23	6.67	-18.48	13.57	-3.41	15.43	12.10
5a	-33.19	-1.60	-18.69	-0.01	-1.60	-39.23	-6.77	-24.15	-5.50	-9.05	-35.33	-3.29	-20.27	-1.42	-4.76

Table S4. $\Delta G°_{RAF}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO•, CH_3O• through RAF in fluoxetine (1).

	$\Delta G°_{gas}$	$\Delta G°_{water}$	$\Delta G°_{benzene}$
Site		HO•	
1	-7.98	-7.80	-6.57
2	-3.40	-4.11	-2.48
3	-8.82	-7.72	-7.40
4	-6.81	-5.68	-5.37
5	-9.20	-6.56	-7.35
6	-8.41	-6.77	-6.59
8	-5.03	-2.64	-2.96
9	-7.62	-5.94	-5.91
10	-5.82	-4.76	-4.00
11	-6.47	-6.55	-5.40
12	-7.53	-6.28	-6.14
13	-8.29	-7.15	-6.88

Table S5. $\Delta G°_{RAF}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO$^{\bullet}$, $CH_3O^{\bullet}$ through RAF in serotonin (**2**).

	$\Delta G°_{gas}$	$\Delta G°_{water}$	$\Delta G°_{benzene}$	$\Delta G°_{gas}$	$\Delta G°_{water}$	$\Delta G°_{benzene}$
Site		HO$^{\bullet}$			$CH_3O^{\bullet}$	
1	-18.95	-19.59	-17.17	-6.58	-6.57	-4.13
2	-11.50	-8.85	-9.22	0.52	2.10	3.35
3	4.66	5.65	6.64	17.27	18.00	19.93
4	-18.88	-14.50	-16.57	-7.17	-3.19	-4.26
5	-10.17	-11.24	-9.31	1.62	2.20	3.48
6	-11.51	-10.34	-10.05	1.64	2.20	3.48
7	-11.75	-11.43	-10.29	2.13	0.65	3.29
8	-2.72	-2.00	-0.43	10.03	10.29	12.81

Table S6. $\Delta G^{\ddagger}_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene for serotonin.

	$\Delta G^{\ddagger}_{gas}$					$\Delta G^{\ddagger}_{water}$					$\Delta G^{\ddagger}_{benzene}$				
Site	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO\bullet$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO\bullet$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2CHOO\bullet$
9	5.61		11.97			0.08		14.14			6.87		11.12		
11	6.35		12.12			6.46		11.44			6.91		12.92		
10	6.86		14.43			7.40		14.08			8.02		15.73		
12	5.40		13.13			5.14		13.10			6.06		14.10		
5a	5.02	16.15	7.29	16.61	13.34	11.23	12.98	5.36	13.07	7.55	6.14	16.78	8.50	17.77	13.20

Table S7. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine (1) and fluoxetine radicals obtained with the HAT mechanism. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

1

E=-1088.0350091 Ha

F	5.571082	-0.926634	0.048242
C	4.711842	-0.006101	0.515030
F	4.841138	0.027890	1.850499
F	5.137925	1.182944	0.054859
C	3.304429	-0.299888	0.096791
C	3.058760	-0.877844	-1.149911
C	1.757923	-1.103574	-1.562614
C	0.685137	-0.753127	-0.732863
C	0.927560	-0.169697	0.513326
C	2.241053	0.050850	0.918589
H	2.434703	0.499925	1.887169
H	0.110974	0.128680	1.159012
O	-0.546486	-1.031320	-1.230946
C	-1.693907	-0.785759	-0.420700
C	-1.980621	0.695636	-0.279875
C	-1.648537	1.581832	-1.304345
C	-1.950768	2.935719	-1.184523
C	-2.590654	3.412148	-0.042974
C	-2.925615	2.529654	0.981665
C	-2.619167	1.176494	0.865877
H	-2.882063	0.474759	1.654987
H	-3.420819	2.896595	1.875675
H	-2.823401	4.468437	0.049953
H	-1.681996	3.620866	-1.982756
H	-1.139284	1.206564	-2.187621
C	-2.832475	-1.531678	-1.120829
C	-4.166946	-1.402859	-0.397325
N	-4.052354	-1.823490	0.993809
H	-3.772217	-2.802728	1.019860
C	-5.302658	-1.659749	1.719830
H	-5.194390	-2.050788	2.734461
H	-6.163938	-2.155615	1.241800
H	-5.531201	-0.591009	1.792578
H	-4.939332	-1.966365	-0.950066
H	-4.483911	-0.352922	-0.396946
H	-2.925629	-1.142654	-2.141186
H	-2.541630	-2.586573	-1.202490
H	-1.539812	-1.223965	0.573192
H	1.538547	-1.560054	-2.521677
H	3.890327	-1.158309	-1.788345

1 site 1

E=-1087.3453038 Ha

F	5.584529	-0.947783	0.000433
C	4.729112	-0.035016	0.487565
F	4.858790	-0.028222	1.822760
F	5.153958	1.161868	0.049418
C	3.319974	-0.319604	0.064577
C	3.077076	-0.872544	-1.201990
C	1.772426	-1.061078	-1.558297
C	0.672334	-0.754500	-0.769035
C	0.935963	-0.198830	0.489653
C	2.254984	0.010394	0.892624
H	2.450730	0.436860	1.870608
H	0.124460	0.086860	1.149052
O	-0.554985	-1.024827	-1.273826
C	-1.698241	-0.788604	-0.452545
C	-1.972320	0.691554	-0.279355
C	-1.640349	1.595622	-1.288228
C	-1.930067	2.949207	-1.138142
C	-2.557077	3.407321	0.017975
C	-2.892075	2.506814	1.026812
C	-2.598180	1.153753	0.880940
H	-2.861832	0.437980	1.657099
H	-3.377601	2.859371	1.931836
H	-2.780081	4.463379	0.134342
H	-1.661698	3.648345	-1.924260
H	-1.141579	1.234290	-2.183276
C	-2.843907	-1.511900	-1.164019
C	-4.173908	-1.388619	-0.431330
N	-4.054889	-1.837304	0.950728
H	-3.782118	-2.818980	0.955940
C	-5.300136	-1.678771	1.686666
H	-5.189315	-2.090356	2.692858
H	-6.167454	-2.159034	1.203746
H	-5.520449	-0.610044	1.781460
H	-4.952657	-1.936101	-0.991049
H	-4.483902	-0.336848	-0.408583
H	-2.938373	-1.100681	-2.175433
H	-2.560559	-2.566659	-1.269228
H	-1.542215	-1.249238	0.530873
H	3.899598	-1.143381	-1.857178

1 site 2

E=-1087.3473724 Ha

F	5.554878	-1.070003	0.176573
C	4.759264	-0.035353	0.480493
F	4.865947	0.188062	1.799390
F	5.268012	1.039288	-0.142351
C	3.340154	-0.295928	0.079342
C	3.031508	-0.851567	-1.145715
C	1.770128	-1.095194	-1.608491
C	0.699046	-0.748791	-0.763116
C	0.952766	-0.177295	0.489081

C	2.265535	0.042509	0.900211
H	2.457191	0.484009	1.873250
H	0.137430	0.115778	1.138240
O	-0.533645	-1.018381	-1.255425
C	-1.678361	-0.782332	-0.435207
C	-1.962201	0.697186	-0.274258
C	-1.638289	1.595836	-1.290476
C	-1.937940	2.948379	-1.150665
C	-2.567258	3.410771	0.002490
C	-2.894455	2.515633	1.018652
C	-2.590447	1.163752	0.883050
H	-2.847613	0.452165	1.665201
H	-3.381659	2.871541	1.921460
H	-2.797964	4.466018	0.110899
H	-1.675437	3.643359	-1.942428
H	-1.137547	1.231833	-2.183330
C	-2.820040	-1.518921	-1.139723
C	-4.150232	-1.398427	-0.406887
N	-4.026925	-1.835575	0.978452
H	-3.749233	-2.815800	0.991092
C	-5.272007	-1.677555	1.714947
H	-5.157522	-2.080468	2.724217
H	-6.137465	-2.166199	1.237171
H	-5.497701	-0.609256	1.801476
H	-4.925967	-1.955048	-0.961733
H	-4.466709	-0.348467	-0.392033
H	-2.918401	-1.116503	-2.154361
H	-2.530249	-2.572815	-1.236396
H	-1.517884	-1.233825	0.551455
H	1.561780	-1.542583	-2.574821

1 site 4

E=-1087.3475927 Ha

F	5.613170	-0.868914	0.021213
C	4.738299	0.002776	0.548789
F	4.852498	-0.056862	1.881402
F	5.142411	1.227775	0.175237
C	3.340088	-0.289385	0.100566
C	3.080131	-0.867721	-1.149226
C	1.776214	-1.089868	-1.557038
C	0.696661	-0.741878	-0.730247
C	0.931984	-0.155785	0.523724
C	2.248278	0.034451	0.867579
H	0.123201	0.151129	1.176763
O	-0.530997	-1.020075	-1.230597
C	-1.681158	-0.782252	-0.419192
C	-1.971225	0.697479	-0.271092
C	-1.648814	1.588704	-1.294319
C	-1.953686	2.941199	-1.166368
C	-2.586543	3.410866	-0.018094
C	-2.912016	2.523209	1.005062
C	-2.602962	1.171337	0.881277
H	-2.858464	0.465605	1.669205
H	-3.401278	2.885004	1.904360
H	-2.820876	4.466179	0.081290
H	-1.692291	3.630580	-1.963354
H	-1.144956	1.218989	-2.183060
C	-2.816735	-1.528655	-1.123052
C	-4.150598	-1.406021	-0.397221
N	-4.031958	-1.831032	0.992219
H	-3.752907	-2.810683	1.014511
C	-5.279731	-1.668136	1.723037
H	-5.168047	-2.061858	2.736220
H	-6.142922	-2.162202	1.246734
H	-5.507072	-0.599416	1.799308
H	-4.922333	-1.969434	-0.950803
H	-4.469975	-0.356847	-0.392581
H	-2.911600	-1.135014	-2.141463
H	-2.523148	-2.582387	-1.209454
H	-1.523991	-1.225319	0.571991
H	1.556771	-1.545700	-2.515957
H	3.909729	-1.150713	-1.790243

1 site 5

E=-1087.3492437 Ha

F	5.476989	-0.931776	0.268115
C	4.599918	0.044543	0.551282
F	4.668864	0.282423	1.869805
F	5.045054	1.150526	-0.068051
C	3.210954	-0.318831	0.121642
C	3.020101	-1.030310	-1.063853
C	1.741774	-1.333308	-1.510528
C	0.624570	-0.925394	-0.768520
C	0.864247	-0.225978	0.400787
C	2.110192	0.098247	0.874758
H	2.245716	0.651810	1.798575
O	-0.602816	-1.246332	-1.235590
C	-1.709961	-0.877591	-0.405569
C	-1.883208	0.624732	-0.338719
C	-1.652553	1.413079	-1.466834
C	-1.857878	2.788572	-1.413793
C	-2.302912	3.384146	-0.235580
C	-2.537815	2.599788	0.891442
C	-2.324555	1.224800	0.842135
H	-2.512028	0.599422	1.711831
H	-2.880156	3.060705	1.813091
H	-2.461878	4.457332	-0.194951
H	-1.667434	3.397537	-2.292301
H	-1.294338	0.943655	-2.379325
C	-2.922422	-1.576725	-1.018513
C	-4.211161	-1.282722	-0.260111
N	-4.070479	-1.607455	1.153857
H	-3.889583	-2.605762	1.246623
C	-5.258389	-1.258183	1.917646

H	-5.139273	-1.583225	2.954170
H	-6.189948	-1.692857	1.518028
H	-5.370133	-0.168655	1.916324
H	-5.051920	-1.814846	-0.739256
H	-4.436130	-0.211414	-0.328239
H	-3.024277	-1.251470	-2.060386
H	-2.722196	-2.655474	-1.034445
H	-1.537065	-1.262206	0.606840
H	1.579874	-1.890124	-2.427916
H	3.883068	-1.355331	-1.635792

1 site 7

E=-1087.3790512 Ha

F	5.498656	-0.817105	-0.080563
C	4.576137	-0.150284	0.631499
F	4.669761	-0.564187	1.904556
F	4.940549	1.143039	0.617062
C	3.198135	-0.352561	0.079378
C	3.019995	-0.514514	-1.293941
C	1.742918	-0.649090	-1.815438
C	0.640306	-0.624037	-0.959422
C	0.809893	-0.464400	0.416230
C	2.095185	-0.328666	0.927335
H	2.240237	-0.211011	1.996150
H	-0.053224	-0.447983	1.071883
O	-0.579069	-0.797869	-1.554334
C	-1.737794	-0.550711	-0.839059
C	-1.987840	0.813615	-0.439447
C	-1.242748	1.860016	-1.029651
C	-1.452318	3.179471	-0.659247
C	-2.398901	3.500118	0.313358
C	-3.125371	2.476724	0.921135
C	-2.925150	1.151025	0.562553
H	-3.439734	0.354243	1.090151
H	-3.845896	2.712936	1.698748
H	-2.559646	4.533900	0.602017
H	-0.875428	3.965645	-1.136923
H	-0.516475	1.625529	-1.800934
C	-2.697146	-1.683278	-1.057973
C	-4.069780	-1.620316	-0.402667
N	-3.986537	-1.804986	1.038089
H	-3.510207	-2.683156	1.233272
C	-5.297888	-1.807227	1.667552
H	-5.194939	-2.022077	2.733743
H	-6.001432	-2.533427	1.227058
H	-5.742143	-0.810687	1.566775
H	-4.716820	-2.376703	-0.881479
H	-4.535561	-0.645972	-0.596018
H	-2.838046	-1.773748	-2.146825
H	-2.195947	-2.617348	-0.762555
H	1.574060	-0.781854	-2.878513
H	3.883016	-0.541461	-1.951159

1 site 9

E=-1087.3484285 Ha

F	5.555592	-0.916733	0.033856
C	4.690206	-0.004767	0.506160
F	4.827691	0.030208	1.840959
F	5.102038	1.188525	0.043881
C	3.283244	-0.312217	0.096861
C	3.034891	-0.891353	-1.148910
C	1.733897	-1.129355	-1.553524
C	0.663005	-0.790269	-0.716671
C	0.908218	-0.206458	0.528822
C	2.221934	0.026991	0.925947
H	2.417406	0.476320	1.894043
H	0.093706	0.081010	1.182014
O	-0.567923	-1.085719	-1.204655
C	-1.714956	-0.811347	-0.408073
C	-1.969617	0.676929	-0.294773
C	-1.604690	1.559291	-1.288887
C	-1.820479	2.917372	-1.269809
C	-2.476007	3.441430	-0.150681
C	-2.873985	2.594960	0.883550
C	-2.621910	1.225871	0.818682
H	-2.934323	0.559390	1.620904
H	-3.378590	3.006286	1.752153
H	-2.670144	4.508191	-0.088342
H	-1.496942	3.560797	-2.082270
C	-2.863718	-1.540351	-1.107835
C	-4.202992	-1.362692	-0.403857
N	-4.112474	-1.741350	1.001250
H	-3.842621	-2.722054	1.061113
C	-5.371860	-1.544397	1.703278
H	-5.281808	-1.904200	2.731140
H	-6.230132	-2.047915	1.228066
H	-5.592415	-0.472098	1.739122
H	-4.980362	-1.927885	-0.947651
H	-4.499465	-0.307283	-0.439866
H	-2.931271	-1.166889	-2.135642
H	-2.598595	-2.603493	-1.165653
H	-1.579839	-1.234037	0.595363
H	1.512186	-1.584615	-2.512497
H	3.864952	-1.162152	-1.793451

1 site 10

E=-1087.3493801 Ha

F	5.530709	-0.990882	0.203734
C	4.704695	0.022517	0.512746
F	4.813979	0.245639	1.831112
F	5.189214	1.110888	-0.109259
C	3.293851	-0.273329	0.107407
C	3.051898	-0.905823	-1.113921

C	1.752828	-1.143677	-1.523576
C	0.677732	-0.751553	-0.715280
C	0.915974	-0.114391	0.504266
C	2.228856	0.119051	0.906616
H	2.419447	0.611486	1.854205
H	0.097741	0.216623	1.131829
O	-0.553417	-1.045632	-1.208060
C	-1.701609	-0.772769	-0.409789
C	-1.993309	0.713015	-0.331685
C	-1.654751	1.554461	-1.399553
C	-1.986853	2.883332	-1.280082
C	-2.623156	3.453484	-0.201411
C	-2.954280	2.599055	0.855898
C	-2.638815	1.243279	0.789615
H	-2.902067	0.572985	1.604967
H	-3.454069	2.996051	1.735034
H	-2.856641	4.512845	-0.161769
H	-1.138978	1.155570	-2.268731
C	-2.838234	-1.550033	-1.078259
C	-4.172899	-1.396852	-0.359742
N	-4.054243	-1.754081	1.048755
H	-3.768790	-2.729693	1.118106
C	-5.304983	-1.565470	1.768349
H	-5.193098	-1.909716	2.799383
H	-6.163424	-2.087789	1.314220
H	-5.540150	-0.495984	1.793141
H	-4.941988	-1.989272	-0.885985
H	-4.496799	-0.350070	-0.405963
H	-2.932973	-1.204216	-2.113864
H	-2.542763	-2.606036	-1.116161
H	-1.547025	-1.166697	0.602303
H	1.535993	-1.640860	-2.462746
H	3.885815	-1.218173	-1.734662

1 site 11

E=-1087.3488937 Ha

F	5.545554	-0.946617	0.047338
C	4.695765	-0.018174	0.515618
F	4.824860	0.012131	1.851093
F	5.133553	1.167166	0.057294
C	3.285491	-0.297238	0.096414
C	3.034699	-0.866636	-1.153221
C	1.731922	-1.079213	-1.566785
C	0.662529	-0.724106	-0.734769
C	0.910014	-0.149298	0.514265
C	2.225462	0.058129	0.920402
H	2.423112	0.500486	1.891238
H	0.096220	0.152230	1.161957
O	-0.571846	-0.989135	-1.234394
C	-1.717305	-0.739619	-0.423003
C	-1.994816	0.743863	-0.277249
C	-1.656294	1.626900	-1.304225
C	-1.946600	2.989882	-1.189737
C	-2.575551	3.402496	-0.037548
C	-2.933699	2.578211	1.004970
C	-2.629496	1.219777	0.874295
H	-2.894863	0.513634	1.659339
H	-3.425252	2.955840	1.896391
H	-1.678114	3.684146	-1.980031
H	-1.150611	1.246937	-2.188121
C	-2.860210	-1.477877	-1.123973
C	-4.194314	-1.340026	-0.401380
N	-4.082328	-1.756267	0.991400
H	-3.805341	-2.736324	1.020992
C	-5.333203	-1.586525	1.715469
H	-5.227287	-1.974663	2.731428
H	-6.195078	-2.081475	1.237802
H	-5.558961	-0.516936	1.784473
H	-4.969230	-1.901585	-0.952367
H	-4.506433	-0.288591	-0.404843
H	-2.950205	-1.088445	-2.144481
H	-2.576381	-2.534657	-1.205403
H	-1.564804	-1.181190	0.569548
H	1.508503	-1.528982	-2.528081
H	3.863736	-1.150886	-1.793263

1 site 12

E=-1087.3494953 Ha

F	5.541761	-0.949786	0.014590
C	4.692107	-0.034895	0.509048
F	4.825385	-0.038363	1.844386
F	5.126606	1.162397	0.079467
C	3.280951	-0.305347	0.087081
C	3.027441	-0.839909	-1.177323
C	1.723813	-1.043962	-1.592528
C	0.656594	-0.714974	-0.747223
C	0.906572	-0.174953	0.516683
C	2.222880	0.024162	0.924262
H	2.422599	0.439509	1.906523
H	0.094329	0.106169	1.175556
O	-0.579108	-0.968337	-1.250320
C	-1.721092	-0.747999	-0.427174
C	-2.001757	0.729660	-0.233863
C	-1.656525	1.654698	-1.220434
C	-1.946502	3.008633	-1.060970
C	-2.594623	3.462558	0.092196
C	-2.916500	2.512053	1.034561
C	-2.649717	1.167374	0.932034
H	-2.930338	0.446541	1.697761
H	-2.823973	4.514571	0.229941
H	-1.663677	3.716493	-1.834903
H	-1.142754	1.307567	-2.112031
C	-2.866720	-1.465109	-1.145890
C	-4.198547	-1.351002	-0.414753

N	-4.079122	-1.800545	0.966905
H	-3.799011	-2.780156	0.971906
C	-5.327241	-1.651719	1.700727
H	-5.215277	-2.063915	2.706474
H	-6.189643	-2.137838	1.215101
H	-5.555443	-0.584814	1.796712
H	-4.972860	-1.902523	-0.976587
H	-4.515806	-0.301460	-0.391150
H	-2.960156	-1.045261	-2.153837
H	-2.581209	-2.518413	-1.259644
H	-1.563914	-1.218965	0.551018
H	1.498226	-1.466927	-2.565411
H	3.855061	-1.103897	-1.827810

1 site 13

E=-1087.3487923 Ha

F	5.536422	-0.939428	0.211778
C	4.693152	0.059745	0.520812
F	4.798808	0.284842	1.838983
F	5.159637	1.155931	-0.101828
C	3.287849	-0.259838	0.114634
C	3.057504	-0.876612	-1.116984
C	1.763250	-1.137050	-1.528058
C	0.681419	-0.784088	-0.710585
C	0.907843	-0.163059	0.519702
C	2.216128	0.093421	0.923141
H	2.397755	0.573203	1.878921
H	0.083596	0.136323	1.155450
O	-0.544045	-1.094851	-1.206825
C	-1.693594	-0.862028	-0.398935
C	-2.018429	0.616237	-0.304602
C	-1.650984	1.516439	-1.311661
C	-1.995226	2.863878	-1.214126
C	-2.713000	3.337865	-0.117779
C	-3.093416	2.457227	0.901469
C	-2.723255	1.140315	0.759982
H	-3.650064	2.806767	1.765848
H	-2.975279	4.389617	-0.049893
H	-1.697149	3.550247	-2.000300
H	-1.082148	1.151407	-2.162891
C	-2.819703	-1.658640	-1.061717
C	-4.155541	-1.482120	-0.348923
N	-4.018253	-1.741598	1.078186
H	-3.819517	-2.730330	1.220277
C	-5.206657	-1.368231	1.828237
H	-5.082832	-1.649498	2.876892
H	-6.137569	-1.823338	1.450401
H	-5.319383	-0.279517	1.782597
H	-4.922108	-2.112791	-0.832015
H	-4.489635	-0.444000	-0.458418
H	-2.907770	-1.338089	-2.106050
H	-2.521757	-2.714372	-1.070385
H	-1.526236	-1.257089	0.608949
H	1.555446	-1.622827	-2.475230
H	3.896939	-1.158601	-1.744887

1 site 14

E=-1087.3669128 Ha

F	5.537433	-0.983430	0.036492
C	4.692578	-0.057210	0.518141
F	4.812911	-0.055527	1.854704
F	5.144168	1.133146	0.086842
C	3.283019	-0.314944	0.083294
C	3.037092	-0.838573	-1.187284
C	1.735992	-1.032111	-1.614987
C	0.663695	-0.703310	-0.775973
C	0.905921	-0.173604	0.493854
C	2.219938	0.014729	0.913924
H	2.413821	0.422017	1.900684
H	0.089469	0.109152	1.146938
O	-0.568848	-0.946422	-1.290911
C	-1.709857	-0.731312	-0.468549
C	-1.994595	0.751452	-0.257759
C	-1.595865	1.694408	-1.204755
C	-1.908281	3.038823	-1.023740
C	-2.628039	3.446987	0.096859
C	-3.033181	2.505008	1.039922
C	-2.716882	1.160213	0.865724
H	-3.031221	0.412372	1.591507
H	-3.591399	2.818758	1.916928
H	-2.869361	4.496153	0.236430
H	-1.586495	3.770267	-1.758842
H	-1.029893	1.370880	-2.073530
C	-2.862220	-1.376624	-1.172198
C	-4.177618	-1.477850	-0.478519
N	-4.015699	-1.946340	0.895519
H	-3.603338	-2.877297	0.872743
C	-5.281323	-1.989347	1.612022
H	-5.125417	-2.411265	2.607710
H	-6.063528	-2.574696	1.100642
H	-5.654703	-0.966919	1.733463
H	-4.867728	-2.105242	-1.069646
H	-4.648588	-0.480499	-0.417333
H	-2.827712	-1.378511	-2.256755
H	-1.560853	-1.207459	0.510643
H	1.516078	-1.447311	-2.592480
H	3.868691	-1.102750	-1.832651

1 site 15

E=-1087.380781 Ha

F	5.534978	-1.007676	0.055677
C	4.698840	-0.065958	0.522391
F	4.819275	-0.044172	1.858828
F	5.161723	1.112948	0.072152

C	3.286980	-0.317539	0.091560
C	3.036273	-0.856049	-1.171892
C	1.733460	-1.044964	-1.596528
C	0.664020	-0.696373	-0.761710
C	0.911323	-0.151628	0.500770
C	2.226929	0.031910	0.917986
H	2.424591	0.451151	1.898984
H	0.096793	0.146783	1.149271
O	-0.571390	-0.936066	-1.271667
C	-1.714830	-0.710563	-0.454287
C	-1.996134	0.762693	-0.254230
C	-1.594670	1.701501	-1.203892
C	-1.902642	3.048419	-1.030708
C	-2.617288	3.465469	0.089303
C	-3.021830	2.530179	1.039458
C	-2.710723	1.184140	0.869596
H	-3.022881	0.446513	1.606517
H	-3.575445	2.850350	1.917003
H	-2.854228	4.516266	0.224166
H	-1.580357	3.774291	-1.771028
H	-1.031352	1.372086	-2.072288
C	-2.878396	-1.425885	-1.172545
C	-4.160915	-1.390601	-0.411324
N	-4.170908	-2.010030	0.837922
H	-3.693924	-2.907215	0.840143
C	-5.431445	-2.037389	1.558918
H	-5.281025	-2.482939	2.544506
H	-6.219182	-2.591632	1.030034
H	-5.774728	-1.008093	1.700343
H	-4.788328	-0.505761	-0.474673
H	-3.009515	-0.958232	-2.153812
H	-2.552609	-2.461120	-1.348422
H	-1.563087	-1.191686	0.522609
H	1.509737	-1.470822	-2.568582
H	3.865512	-1.135274	-1.813987

1 site 16

E=-1087.3758371 Ha

F	5.557661	-0.899556	0.183128
C	4.703922	0.091147	0.490156
F	4.827547	0.339428	1.802727
F	5.142757	1.184647	-0.156985
C	3.297250	-0.256738	0.113158
C	3.056382	-0.917145	-1.093581
C	1.759412	-1.203225	-1.477916
C	0.684792	-0.832591	-0.658661
C	0.922154	-0.169149	0.546904
C	2.232934	0.113356	0.923792
H	2.422539	0.625774	1.860931
H	0.104218	0.142200	1.184515
O	-0.542855	-1.174537	-1.126697
C	-1.691472	-0.900814	-0.329321
C	-2.012395	0.579816	-0.288518
C	-1.791277	1.381464	-1.408265
C	-2.140205	2.729046	-1.385231
C	-2.717413	3.284217	-0.245384
C	-2.938908	2.488103	0.876033
C	-2.583942	1.141826	0.855122
H	-2.750320	0.513774	1.728656
H	-3.379753	2.917502	1.770660
H	-2.987364	4.335522	-0.228720
H	-1.957950	3.348479	-2.258086
H	-1.331039	0.944983	-2.290509
C	-2.815573	-1.718187	-0.969736
C	-4.163037	-1.492582	-0.294969
N	-4.085776	-1.726042	1.127378
C	-5.310734	-1.350715	1.784865
H	-5.282328	-1.639494	2.837425
H	-6.190317	-1.809836	1.307333
H	-5.450854	-0.259107	1.721897
H	-4.916122	-2.170693	-0.730863
H	-4.527031	-0.470518	-0.494427
H	-2.880321	-1.445705	-2.029466
H	-2.537950	-2.775495	-0.911189
H	-1.528976	-1.270548	0.691148
H	1.543809	-1.722967	-2.405070
H	3.889993	-1.212935	-1.722815

1 site 17

E=-1087.3786601 Ha

F	5.510787	-0.949815	0.184893
C	4.674653	0.054047	0.497817
F	4.787672	0.278664	1.815433
F	5.143614	1.147485	-0.127420
C	3.265572	-0.258170	0.098583
C	3.025636	-0.871109	-1.133204
C	1.728099	-1.125444	-1.537403
C	0.652350	-0.769970	-0.712963
C	0.888460	-0.152836	0.517121
C	2.200064	0.097809	0.913778
H	2.389025	0.575207	1.869313
H	0.069302	0.150500	1.157259
O	-0.576618	-1.078972	-1.201761
C	-1.724514	-0.838722	-0.392703
C	-2.041374	0.638675	-0.278590
C	-1.748574	1.507264	-1.329893
C	-2.082033	2.855805	-1.237375
C	-2.715028	3.344178	-0.096853
C	-3.010814	2.479479	0.954457
C	-2.672074	1.131825	0.866074
H	-2.904120	0.449432	1.681625
H	-3.500396	2.855281	1.847752
H	-2.972824	4.396270	-0.025583
H	-1.843747	3.527531	-2.056367

H	-1.245178	1.122613	-2.212520
C	-2.850736	-1.620803	-1.073818
C	-4.189394	-1.498362	-0.357102
N	-4.077845	-1.902961	1.037457
H	-3.763386	-2.863122	1.140651
C	-5.120078	-1.563301	1.894747
H	-5.066820	-1.973352	2.896288
H	-5.512299	-0.558350	1.774201
H	-4.953938	-2.079638	-0.893455
H	-4.519290	-0.453772	-0.362032
H	-2.952458	-1.256678	-2.102386
H	-2.542226	-2.672045	-1.133532
H	-1.557017	-1.253760	0.609759
H	1.513010	-1.607967	-2.484594
H	3.860275	-1.154856	-1.766671

Table S8. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine metabolites M1 and all their radicals obtained with the HAT mechanism. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

M1

E=-1048.7363412 Ha

F	-5.222455	-0.184624	0.909677
F	-5.155883	0.866331	-0.968188
F	-4.711232	-1.243009	-0.909796
O	0.843797	1.303889	0.629990
N	5.370965	2.461258	-0.340484
C	1.909086	0.864511	-0.206987
C	3.092030	1.761535	0.152030
C	2.221165	-0.604015	0.000490
C	4.330522	1.500891	-0.697113
C	-0.423532	0.895582	0.363206
C	2.660532	-1.390983	-1.064563
C	2.116195	-1.169619	1.271448
C	-1.410406	1.433300	1.199678
C	-0.779303	0.012464	-0.658483
C	2.999908	-2.726420	-0.862792
C	2.448468	-2.505751	1.472829
C	-3.098633	0.222288	-0.015085
C	-2.738826	1.098737	1.010708
C	-2.120584	-0.315164	-0.840842
C	2.893124	-3.286092	0.407563
C	-4.545102	-0.088930	-0.246043
H	1.632797	1.033794	-1.259322
H	3.341714	1.621352	1.209072
H	2.768892	2.802869	0.028430
H	4.050482	1.515697	-1.766685
H	4.711498	0.496320	-0.486416
H	2.734595	-0.954619	-2.059240
H	1.760664	-0.558004	2.095980
H	-1.102629	2.111936	1.987674
H	-0.028416	-0.439938	-1.294005
H	3.339628	-3.330465	-1.698448
H	2.358197	-2.940306	2.463576
H	5.089907	3.394597	-0.633784
H	6.227904	2.248818	-0.844643
H	-3.503327	1.511229	1.661441
H	-2.401164	-1.006903	-1.628045
H	3.150393	-4.328592	0.566392

M1 site 1

E=-1048.0464807 Ha

F	-5.235172	-0.172690	0.926104
F	-5.166090	0.910448	-0.933471
F	-4.725522	-1.200623	-0.911502
O	0.854655	1.315297	0.667950
N	5.388835	2.453540	-0.291838
C	1.915908	0.881903	-0.179645
C	3.105789	1.763195	0.193806
C	2.214559	-0.592601	0.001758
C	4.339263	1.509721	-0.664903
C	-0.408344	0.909615	0.392250
C	2.641793	-1.365654	-1.078253
C	2.107918	-1.178320	1.263506
C	-1.426829	1.395309	1.201267
C	-0.785272	0.046029	-0.643560
C	2.967579	-2.707918	-0.900374
C	2.426592	-2.521170	1.440763
C	-3.111375	0.246341	0.009241
C	-2.753357	1.105592	1.059708
C	-2.131499	-0.273059	-0.825767
C	2.859062	-3.287890	0.360667
C	-4.559333	-0.058736	-0.228197
H	1.638259	1.072528	-1.228006
H	3.357535	1.600069	1.246995
H	2.789840	2.809004	0.091983
H	4.055757	1.549254	-1.732977
H	4.712358	0.497776	-0.476435
H	2.717532	-0.913065	-2.065538
H	1.762044	-0.576941	2.099644
H	-0.040263	-0.399046	-1.292780
H	3.298140	-3.301167	-1.747338
H	2.335332	-2.971549	2.424304
H	5.114387	3.395360	-0.563398
H	6.242178	2.245096	-0.803663
H	-3.507378	1.511185	1.727813
H	-2.414256	-0.948418	-1.625897
H	3.105772	-4.335607	0.500779

M1 site 2

E=-1048.0486244 Ha

F	-5.176603	-0.389385	0.945426
F	-5.260358	0.994756	-0.700159
F	-4.764242	-1.074456	-1.066583
O	0.836191	1.312068	0.642621
N	5.375509	2.432894	-0.313988
C	1.898878	0.869273	-0.199044
C	3.089260	1.752234	0.169182
C	2.195471	-0.603716	-0.003719
C	4.326171	1.486390	-0.680835
C	-0.432714	0.917495	0.377402
C	2.621924	-1.386778	-1.076804
C	2.089649	-1.177882	1.263362
C	-1.415838	1.460800	1.226202
C	-0.802213	0.045686	-0.652488
C	2.947463	-2.727402	-0.886820
C	2.407866	-2.519150	1.452791
C	-3.133106	0.252724	-0.017052
C	-2.710870	1.101782	0.986261
C	-2.144258	-0.277849	-0.843017
C	2.839510	-3.295820	0.379518
C	-4.585803	-0.056968	-0.210586
H	1.623157	1.051176	-1.249171
H	3.336443	1.600446	1.225188
H	2.776544	2.797685	0.054044
H	4.047815	1.513422	-1.750593
H	4.696470	0.476174	-0.478320
H	2.697049	-0.943366	-2.068262
H	1.744646	-0.569211	2.094543
H	-1.117454	2.134732	2.022475
H	-0.053824	-0.404479	-1.291977
H	3.277321	-3.328464	-1.728519
H	2.316878	-2.960460	2.440449
H	5.106151	3.371285	-0.601995
H	6.232255	2.214252	-0.815761
H	-2.424972	-0.960854	-1.638523
H	3.085908	-4.342286	0.529097

M1 site 4

E=-1048.0488696 Ha

F	5.312256	-0.028191	0.838354
F	5.118689	-0.693008	-1.202884
F	4.714586	1.364871	-0.710561
O	-0.831110	-1.298806	0.628451
N	-5.361363	-2.453835	-0.333101
C	-1.898098	-0.861750	-0.210178
C	-3.080815	-1.756730	0.153495
C	-2.207463	0.607801	-0.008532
C	-4.319976	-1.496664	-0.694992
C	0.433726	-0.893275	0.359765
C	-2.636725	1.392579	-1.079237
C	-2.109609	1.176645	1.261598
C	1.425920	-1.431953	1.192936
C	0.785902	-0.004987	-0.668879
C	-2.973003	2.729785	-0.883867
C	-2.438773	2.514463	1.456403
C	3.135632	-0.228921	-0.017228
C	2.758602	-1.105672	1.008737
C	2.124745	0.273036	-0.799329
C	-2.873193	3.292863	0.385469
C	4.572250	0.107340	-0.273359
H	-1.620656	-1.036268	-1.261286
H	-3.329128	-1.612533	1.210314
H	-2.759325	-2.798894	0.032838
H	-4.041554	-1.515621	-1.764872
H	-4.698563	-0.490637	-0.487027
H	-2.705139	0.953533	-2.073118
H	-1.762047	0.566674	2.090775
H	1.116398	-2.109562	1.980606
H	0.044780	0.460136	-1.308260
H	-3.304284	3.332447	-1.723822
H	-2.353937	2.951926	2.446315
H	-5.084227	-3.388351	-0.626328
H	-6.219905	-2.239613	-0.833723
H	3.519136	-1.523146	1.661532
H	-3.127634	4.336792	0.539168

M1 site 5

E=-1048.051295 Ha

F	-5.139724	-0.133504	0.882306
F	-5.054841	0.829031	-1.042054
F	-4.563050	-1.263862	-0.873360
O	0.925965	1.446258	0.641255
N	5.528631	2.125096	-0.490962
C	1.934612	0.899033	-0.213418
C	3.202070	1.690262	0.087220
C	2.108421	-0.587209	0.015504
C	4.380914	1.271092	-0.783613
C	-0.342571	1.042604	0.403557
C	2.225471	-1.462614	-1.063402
C	2.193274	-1.086908	1.316477
C	-1.366084	1.581479	1.195500
C	-0.711512	0.135526	-0.573639
C	2.438326	-2.822236	-0.848625
C	2.396611	-2.445554	1.532501
C	-3.005174	0.278584	-0.015994
C	-2.682834	1.199948	0.981755
C	-1.999043	-0.273994	-0.812548
C	2.523615	-3.315146	0.450303
C	-4.440459	-0.076146	-0.261946
H	1.631637	1.065226	-1.258582
H	3.469939	1.563710	1.141722

H	2.981683	2.754023	-0.067318
H	4.071545	1.277807	-1.844791
H	4.656842	0.238725	-0.544533
H	2.142659	-1.075629	-2.076945
H	2.083656	-0.405066	2.155748
H	-1.101051	2.292226	1.971622
H	2.527437	-3.496470	-1.694792
H	2.455392	-2.828524	2.546633
H	5.340373	3.072264	-0.812901
H	6.341832	1.803468	-1.009637
H	-3.472055	1.613654	1.600964
H	-2.236040	-1.003120	-1.580917
H	2.682744	-4.375355	0.620595

M1 site 7

E=-1048.0886927 Ha

F	-5.330236	-0.008712	0.616714
F	-4.707552	0.766960	-1.307181
F	-4.928713	-1.355838	-1.019083
O	0.878703	-0.721486	1.139659
N	1.644993	3.885431	-0.028167
C	1.822878	0.169631	0.679606
C	1.594503	1.630167	0.917555
C	3.030769	-0.390241	0.182680
C	1.430508	2.478010	-0.354352
C	-0.420065	-0.552058	0.739180
C	4.146300	0.432187	-0.116204
C	3.155355	-1.785175	-0.031852
C	-1.419455	-0.799090	1.677636
C	-0.739765	-0.197411	-0.572145
C	5.316134	-0.119925	-0.611730
C	4.332213	-2.319998	-0.526405
C	-3.077995	-0.312843	0.000019
C	-2.751611	-0.681521	1.302877
C	-2.073977	-0.074494	-0.936345
C	5.420841	-1.495942	-0.823067
C	-4.513723	-0.225800	-0.424629
H	2.446724	2.048517	1.470461
H	0.713305	1.749327	1.558968
H	0.449442	2.262357	-0.805545
H	2.191457	2.180334	-1.083805
H	4.089951	1.503769	0.052378
H	2.312777	-2.427444	0.199171
H	-1.133851	-1.075341	2.686582
H	0.058240	-0.038602	-1.290847
H	6.159302	0.527861	-0.831966
H	4.406373	-3.391826	-0.684335
H	0.900046	4.209380	0.586180
H	1.580611	4.450294	-0.871510
H	-3.539754	-0.862243	2.025896
H	-2.338422	0.204425	-1.951410
H	6.340282	-1.921607	-1.211325

M1 site 9

E=-1048.0493768 Ha

F	-5.194150	-0.197708	0.921351
F	-5.141604	0.886348	-0.938047
F	-4.691119	-1.222368	-0.919623
O	0.865622	1.316736	0.626292
N	5.416670	2.416592	-0.304356
C	1.930724	0.874351	-0.204892
C	3.123629	1.749907	0.170162
C	2.222359	-0.597580	0.000339
C	4.363024	1.475831	-0.673484
C	-0.400866	0.905721	0.363315
C	2.638256	-1.424793	-1.050336
C	2.135376	-1.187292	1.243839
C	-1.383314	1.422652	1.217962
C	-0.761965	0.043063	-0.673863
C	2.945972	-2.764790	-0.820356
C	2.415974	-2.502897	1.525176
C	-3.076853	0.231177	-0.008973
C	-2.711860	1.087678	1.031914
C	-2.103422	-0.285786	-0.852853
C	2.835226	-3.306523	0.458853
C	-4.523831	-0.079727	-0.236366
H	1.667329	1.048299	-1.259866
H	3.359934	1.594674	1.227933
H	2.816785	2.796767	0.052394
H	4.089668	1.502395	-1.744679
H	4.727105	0.463900	-0.467425
H	2.716938	-1.011688	-2.055050
H	-1.070967	2.084035	2.018580
H	-0.015546	-0.391889	-1.326544
H	3.265845	-3.391491	-1.646610
H	2.318870	-2.908102	2.527659
H	5.151628	3.356646	-0.590925
H	6.272701	2.194916	-0.806042
H	-3.472628	1.483700	1.697071
H	-2.387697	-0.961706	-1.652388
H	3.069649	-4.352890	0.630296

M1 site 10

E=-1048.0504941 Ha

F	-5.212851	-0.158364	0.910371
F	-5.135027	0.843216	-0.993809
F	-4.700322	-1.266082	-0.879058
O	0.860386	1.296113	0.616440
N	5.390617	2.416168	-0.382830
C	1.925429	0.831241	-0.204871
C	3.110609	1.735433	0.127865
C	2.234233	-0.631331	0.049837
C	4.350270	1.445827	-0.710360

C	-0.408582	0.886232	0.355174
C	2.681134	-1.454491	-0.986077
C	2.116920	-1.153284	1.345083
C	-1.396578	1.455036	1.169072
C	-0.762846	-0.026879	-0.640017
C	3.021181	-2.785596	-0.750164
C	2.460633	-2.471804	1.522670
C	-3.084346	0.215033	-0.016828
C	-2.725630	1.121220	0.983236
C	-2.104906	-0.353284	-0.819723
C	2.911001	-3.320632	0.536837
C	-4.531517	-0.095924	-0.245027
H	1.651382	0.966166	-1.262667
H	3.357936	1.628630	1.189305
H	2.789499	2.772781	-0.029345
H	4.072054	1.425925	-1.780360
H	4.730064	0.448373	-0.466349
H	2.761481	-1.047608	-1.992139
H	1.756090	-0.526526	2.156050
H	-1.089534	2.156362	1.937225
H	-0.010947	-0.503162	-1.256736
H	3.365067	-3.410472	-1.569331
H	5.112781	3.339621	-0.708559
H	6.249726	2.185139	-0.874891
H	-3.491479	1.557499	1.616626
H	-2.384894	-1.068013	-1.586299
H	3.165130	-4.356508	0.737993

M1 site 11

E=-1048.0499964 Ha

F	-5.204348	-0.156770	0.910374
F	-5.127474	0.883490	-0.973046
F	-4.705142	-1.230161	-0.903618
O	0.876719	1.266870	0.622236
N	5.413640	2.374651	-0.360260
C	1.938275	0.809869	-0.209683
C	3.128221	1.701589	0.138658
C	2.237625	-0.659603	0.014498
C	4.365360	1.418973	-0.705499
C	-0.395144	0.870156	0.357493
C	2.662117	-1.460668	-1.047600
C	2.134644	-1.201748	1.297545
C	-1.376334	1.424418	1.189705
C	-0.759873	-0.016342	-0.657922
C	2.995072	-2.802973	-0.839856
C	2.454621	-2.542322	1.526897
C	-3.076964	0.222891	-0.017206
C	-2.708186	1.102738	1.002487
C	-2.104566	-0.330943	-0.838658
C	2.874277	-3.281632	0.444091
C	-4.526826	-0.074454	-0.246145
H	1.663357	0.969224	-1.263822
H	3.375921	1.573699	1.197771
H	2.814191	2.743876	0.000852
H	4.086604	1.421811	-1.775567
H	4.737537	0.414070	-0.480856
H	2.731576	-1.034807	-2.047629
H	1.790048	-0.572032	2.113686
H	-1.061653	2.105468	1.972877
H	-0.013862	-0.481032	-1.290247
H	3.324421	-3.430293	-1.662324
H	2.369929	-2.972578	2.519951
H	5.142155	3.306409	-0.667185
H	6.270040	2.147092	-0.858657
H	-3.468450	1.528067	1.649900
H	-2.392273	-1.025219	-1.621030

M1 site 12

E=-1048.0504741 Ha

F	-5.194097	-0.203389	0.912527
F	-5.132989	0.922036	-0.921716
F	-4.703015	-1.191147	-0.951622
O	0.879832	1.256288	0.649479
N	5.411940	2.405472	-0.307264
C	1.937199	0.834848	-0.204658
C	3.130309	1.709601	0.175212
C	2.238168	-0.642617	-0.041562
C	4.364102	1.461553	-0.684726
C	-0.392585	0.866475	0.375672
C	2.673791	-1.399168	-1.138362
C	2.127667	-1.248774	1.211205
C	-1.371077	1.386937	1.232428
C	-0.759424	0.017302	-0.670251
C	2.982908	-2.720312	-0.913353
C	2.446513	-2.593806	1.383124
C	-3.074077	0.226281	-0.010565
C	-2.702923	1.068717	1.039434
C	-2.104169	-0.294106	-0.856421
C	2.889665	-3.361221	0.300267
C	-4.524379	-0.065968	-0.243401
H	1.658257	1.035971	-1.250553
H	3.381283	1.538053	1.227238
H	2.816045	2.756687	0.081256
H	4.080842	1.505129	-1.752682
H	4.739221	0.449599	-0.500685
H	2.756882	-0.946807	-2.124968
H	1.775666	-0.657756	2.051590
H	-1.054383	2.039272	2.038880
H	-0.015400	-0.421506	-1.323233
H	2.348825	-3.051117	2.363449
H	5.138793	3.347276	-0.580165
H	6.267451	2.196881	-0.815390
H	-3.461350	1.467731	1.705507
H	-2.393623	-0.959503	-1.662819

H	3.140051	-4.410450	0.420621

M1 site 13

E=-1048.0512153 Ha

F	-5.200801	-0.206494	0.893210
F	-5.134253	0.882172	-0.962983
F	-4.686418	-1.227361	-0.946668
O	0.863830	1.295260	0.649546
N	5.379059	2.469952	-0.381354
C	1.925151	0.870979	-0.197118
C	3.113376	1.760971	0.158044
C	2.237155	-0.599993	-0.002491
C	4.345416	1.488117	-0.697575
C	-0.404130	0.892099	0.372731
C	2.734875	-1.383046	-1.021431
C	2.071448	-1.227098	1.238646
C	-1.392758	1.417263	1.214636
C	-0.755893	0.023176	-0.662402
C	3.082757	-2.709473	-0.919589
C	2.402687	-2.570841	1.398101
C	-3.076918	0.222343	-0.021485
C	-2.720525	1.084308	1.017607
C	-2.096593	-0.302496	-0.852687
C	2.906571	-3.312711	0.330485
C	-4.522814	-0.086575	-0.259919
H	1.645492	1.043400	-1.246709
H	3.364593	1.624285	1.215087
H	2.795693	2.803449	0.030291
H	4.052768	1.464423	-1.763303
H	4.740014	0.494798	-0.461372
H	1.668347	-0.652363	2.068549
H	-1.087400	2.085133	2.012716
H	-0.003246	-0.418576	-1.303763
H	3.470458	-3.270049	-1.764544
H	2.263327	-3.045146	2.364232
H	5.087498	3.389815	-0.705444
H	6.234274	2.247762	-0.884284
H	-3.487050	1.487002	1.672089
H	-2.374761	-0.982657	-1.650708
H	3.160358	-4.360005	0.464917

M1 site 14

E=-1048.0686171 Ha

F	-5.194359	-0.202589	0.888572
F	-5.119827	0.911592	-0.951926
F	-4.682876	-1.200396	-0.964670
O	0.876632	1.274905	0.673366
N	5.205079	2.781826	-0.329722
C	1.937299	0.844849	-0.170228
C	3.131263	1.660890	0.197822
C	2.242160	-0.638153	0.006204
C	4.337783	1.658023	-0.675094
C	-0.391563	0.879065	0.390649
C	2.767493	-1.373453	-1.056623
C	2.065940	-1.251341	1.246847
C	-1.380603	1.408304	1.229821
C	-0.744868	0.015667	-0.648472
C	3.115532	-2.710690	-0.882708
C	2.406640	-2.589281	1.417699
C	-3.067174	0.228176	-0.017391
C	-2.709475	1.084623	1.025988
C	-2.086821	-0.300718	-0.845760
C	2.934223	-3.321102	0.355385
C	-4.514215	-0.070168	-0.261924
H	1.670686	1.030505	-1.224099
H	3.254666	1.924239	1.244063
H	4.019400	1.632003	-1.734977
H	4.915652	0.732539	-0.515975
H	2.898019	-0.897679	-2.027220
H	1.650937	-0.675805	2.069255
H	-1.074336	2.072176	2.030845
H	0.007828	-0.430862	-1.286309
H	3.519907	-3.276927	-1.716104
H	2.259129	-3.063568	2.383080
H	4.732152	3.653872	-0.555059
H	6.052638	2.753208	-0.890357
H	-3.476183	1.490551	1.678297
H	-2.365961	-0.976923	-1.646764
H	3.198722	-4.364968	0.491377

M1 site 15

E=-1048.08359 Ha

F	-5.162779	-0.402466	0.894336
F	-5.153240	0.618624	-1.001051
F	-4.569824	-1.455050	-0.903634
O	0.794544	1.478765	0.621241
N	5.075539	0.990517	-0.708558
C	1.892274	1.100952	-0.206983
C	3.017925	2.093893	0.158902
C	2.294117	-0.340353	0.026785
C	4.211230	2.085663	-0.731026
C	-0.441523	0.984231	0.355541
C	2.812048	-1.112423	-1.013574
C	2.188730	-0.895160	1.303145
C	-1.466339	1.464212	1.181605
C	-0.732667	0.067545	-0.657247
C	3.221428	-2.422216	-0.782367
C	2.596177	-2.206152	1.535108
C	-3.063959	0.128820	-0.025163
C	-2.768586	1.039226	0.991450
C	-2.047955	-0.351310	-0.840788
C	3.113461	-2.972062	0.493075
C	-4.484912	-0.281357	-0.258922
H	1.620190	1.249044	-1.261923

H	3.306064	1.881944	1.199475
H	2.568953	3.092708	0.149202
H	4.174720	2.621342	-1.674422
H	2.909366	-0.675844	-2.004485
H	1.770799	-0.297314	2.108524
H	-1.208652	2.171149	1.962704
H	0.050570	-0.339604	-1.284367
H	3.622405	-3.014555	-1.599049
H	2.503631	-2.631986	2.529532
H	5.137155	0.520008	0.188362
H	5.996599	1.166094	-1.093834
H	-3.562124	1.407111	1.634137
H	-2.277907	-1.069151	-1.621015
H	3.427003	-3.995715	0.673030

M1 site 16

E=-1048.0681394 Ha

F	-5.185432	-0.216924	0.918071
F	-5.134657	0.809541	-0.973959
F	-4.661992	-1.292681	-0.887713
O	0.861073	1.344194	0.612786
N	5.373507	2.532934	-0.385805
C	1.929969	0.912272	-0.221594
C	3.100871	1.826974	0.132135
C	2.260829	-0.551136	-0.003096
C	4.346095	1.571847	-0.707475
C	-0.401907	0.917375	0.351608
C	2.692909	-1.346876	-1.064758
C	2.181346	-1.102075	1.276300
C	-1.393283	1.447593	1.187234
C	-0.748201	0.023164	-0.663409
C	3.050568	-2.675891	-0.851743
C	2.531926	-2.431706	1.489180
C	-3.068205	0.205518	-0.014552
C	-2.717574	1.093747	1.004226
C	-2.085409	-0.323994	-0.839741
C	2.969771	-3.220346	0.427099
C	-4.510876	-0.127628	-0.239640
H	1.651974	1.070408	-1.275524
H	3.343727	1.694332	1.192338
H	2.783022	2.865795	-0.002805
H	4.100575	1.618961	-1.784332
H	4.722384	0.548431	-0.540203
H	2.744416	-0.923531	-2.066611
H	1.829943	-0.484500	2.098225
H	-1.092576	2.135996	1.969448
H	0.006707	-0.422611	-1.298850
H	3.383503	-3.286856	-1.685067
H	2.461027	-2.854929	2.486365
H	6.171364	2.323889	-1.000383
H	-3.485803	1.500354	1.654220
H	-2.358823	-1.024485	-1.621708
H	3.241183	-4.257790	0.595000

Table S9. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine metabolites M2 and all their radicals obtained with the HAT mechanism. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

M2

E=-644.4765945 Ha

F	-2.396684	1.233224	-0.004216
F	-2.350105	-0.646924	-1.072603
F	-2.349869	-0.639302	1.077272
O	3.765152	0.064486	0.000219
C	2.409441	0.011285	0.000046
C	1.722457	1.225796	-0.000018
C	1.705390	-1.195847	-0.000042
C	-0.369176	0.029566	-0.000341
C	0.334865	1.230892	-0.000239
C	0.318206	-1.181882	-0.000206
C	-1.866753	0.002297	0.000001
H	2.293240	2.147624	0.000022
H	2.244313	-2.140028	-0.000004
H	-0.205115	2.171222	-0.000410
H	-0.234901	-2.116421	-0.000362
H	4.124597	-0.833913	-0.000289

M2 site 1

E=-643.7861352 Ha

F	-2.394581	1.217823	-0.002495
F	-2.313108	-0.659632	-1.073776
F	-2.313067	-0.655148	1.076507
O	3.810067	0.165972	0.000158
C	2.458399	0.080162	0.000082
C	1.701067	1.237591	0.000001
C	1.759964	-1.134429	0.000014
C	-0.345909	0.053294	-0.000199
C	0.332221	1.277349	-0.000144
C	0.369862	-1.141156	-0.000108
C	-1.844111	-0.003575	0.000000
H	2.310570	-2.072799	0.000052
H	-0.215287	2.214199	-0.000250
H	-0.164445	-2.086230	-0.000200
H	4.186465	-0.725752	-0.000866

M2 site 2

E=-643.7886669 Ha

F	-2.410117	1.198362	-0.006332

F	-2.363468	-0.682664	-1.072162
F	-2.363439	-0.671325	1.078929
O	3.770196	0.048946	0.000292
C	2.416981	-0.015204	0.000048
C	1.718728	1.196302	-0.000016
C	1.720150	-1.233461	-0.000037
C	-0.386639	0.003406	-0.000379
C	0.331088	1.204306	-0.000225
C	0.351944	-1.157743	-0.000236
C	-1.884836	-0.035398	-0.000012
H	2.287185	2.119182	-0.000006
H	2.247986	-2.184099	0.000046
H	-0.208209	2.145988	-0.000455
H	4.140191	-0.845253	-0.000696

M2 site 4

E=-643.7884498 Ha

F	-2.378877	1.277889	-0.004988
F	-2.374967	-0.605004	-1.072524
F	-2.374876	-0.596154	1.077722
O	3.768602	0.092104	-0.000080
C	2.414768	0.040294	0.000135
C	1.727835	1.261683	0.000107
C	1.708219	-1.169009	-0.000033
C	-0.385657	0.037994	-0.000231
C	0.359017	1.195048	-0.000203
C	0.320332	-1.168762	0.000014
C	-1.883001	0.036809	-0.000025
H	2.284034	2.192907	-0.000067
H	2.252206	-2.109809	-0.000275
H	-0.224980	-2.108692	-0.000308
H	4.129335	-0.806156	0.000825

M2 site 5

E=-643.7888538 Ha

F	-2.348974	1.245838	-0.009090
F	-2.336165	-0.639369	-1.069946
F	-2.335312	-0.622883	1.080126
O	3.810551	-0.043295	0.000388
C	2.455780	-0.048331	0.000151
C	1.774866	1.172030	-0.000100
C	1.687027	-1.199173	-0.000108
C	-0.344151	0.005123	-0.000768
C	0.383726	1.191418	-0.000546
C	0.319507	-1.229128	-0.000591
C	-1.843236	0.005490	0.000023
H	2.354042	2.089778	-0.000006
H	-0.141625	2.139660	-0.000819
H	-0.239444	-2.160774	-0.001033
H	4.125557	-0.959143	0.000582

M2 site 6a

E=-643.821551 Ha

F	-2.339356	1.237153	-0.005094
F	-2.280219	-0.642926	-1.073884
F	-2.279565	-0.633572	1.079805
O	3.751840	-0.021672	0.000266
C	2.503492	-0.006730	0.000244
C	1.765427	1.241015	-0.000110
C	1.733555	-1.237683	-0.000123
C	-0.308105	0.032718	-0.000529
C	0.390214	1.249270	-0.000419
C	0.364104	-1.206797	-0.000431
C	-1.812012	0.008418	0.000018
H	2.346833	2.156731	-0.000067
H	2.291593	-2.167821	-0.000110
H	-0.163752	2.181269	-0.000623
H	-0.217177	-2.123966	-0.000671

Table S10. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine serotonin (2) and all serotonin radicals obtained with the HAT mechanism. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

2

E=-572.9358822 Ha

C	-2.308929	-0.914481	0.013350
C	-0.973236	-1.031824	-0.325884
C	-0.168314	0.121117	-0.306095
C	-0.741863	1.359125	0.058253
C	-2.092925	1.474015	0.400814
C	-2.866510	0.330141	0.375584
C	1.219855	0.361101	-0.602428
C	1.426195	1.700281	-0.401400
N	0.256283	2.307371	-0.006104
C	2.240900	-0.666269	-0.986666
H	-0.554800	-1.997179	-0.605023
H	-2.526787	2.429881	0.678573
H	-3.919886	0.359405	0.631582
H	2.336378	2.273243	-0.515619
H	0.142265	3.290320	0.180694
C	2.701681	-1.497990	0.214968
H	1.828197	-1.334573	-1.752848
H	3.119377	-0.174017	-1.416776
N	3.367448	-0.627508	1.179731
H	1.832884	-2.040312	0.626522

H	3.423756	-2.248803	-0.124059
H	3.667719	-1.169430	1.986346
H	2.688594	0.050018	1.523401
O	-3.167762	-1.979617	0.021969
H	-2.682841	-2.771947	-0.246914

2 site 1

E=-572.2399112 Ha

O	3.109262	-2.018404	0.056771
C	2.275714	-0.935394	0.029275
C	2.859342	0.301137	0.371566
C	2.110165	1.462912	0.376978
C	0.760126	1.370110	0.033109
C	0.158316	0.139157	-0.310483
C	0.936737	-1.030224	-0.310745
H	0.497022	-1.990692	-0.572350
C	-1.235877	0.385385	-0.618056
C	-1.378990	1.723723	-0.418183
N	-0.224640	2.345399	-0.050237
H	-0.115271	3.324340	0.159631
C	-2.263841	-0.639173	-0.982575
H	-1.839201	-1.346083	-1.707388
H	-3.112361	-0.150862	-1.476641
C	-2.775403	-1.409246	0.250931
N	-3.435429	-0.593457	1.261476
H	-4.238241	-0.125074	0.843720
H	-2.798497	0.148917	1.547988
H	-1.931223	-1.918183	0.731170
H	-3.475365	-2.187761	-0.071809
H	2.563197	2.413672	0.640276
H	3.912487	0.312325	0.629440
H	2.606098	-2.807286	-0.187778

2 site 4

E=-572.2487411 Ha

O	2.946316	-2.132444	-0.143506
C	2.181495	-1.001611	-0.082887
C	2.820997	0.197902	0.308778
C	2.119602	1.385726	0.402637
C	0.752898	1.379210	0.098692
C	0.077689	0.197332	-0.303445
C	0.844376	-0.956514	-0.373825
C	-1.301255	0.541749	-0.537162
C	-1.405349	1.878234	-0.263563
N	-0.183180	2.389270	0.112024
H	-0.001684	3.350141	0.353706
H	-2.274996	2.518809	-0.317683
C	-2.383549	-0.403712	-0.959204
H	-2.172378	-0.795790	-1.963230
H	-3.335423	0.139304	-1.024576
C	-2.534527	-1.584302	0.016807
N	-2.819372	-1.223923	1.400008
H	-3.669462	-0.662984	1.433504
H	-2.073332	-0.617589	1.738476
H	-1.607766	-2.171425	0.009908
H	-3.330234	-2.248238	-0.338198
H	2.621605	2.298511	0.707629
H	3.881421	0.153539	0.535749
H	2.375321	-2.866250	-0.412437

2 site 5a

E=-572.293544 Ha

O	3.043177	-2.105654	-0.006114
C	2.346125	-1.067913	0.008792
C	2.931390	0.221782	0.379939
C	2.203371	1.373369	0.403700
C	0.831870	1.291753	0.054556
C	0.201606	0.071730	-0.313998
C	0.943981	-1.097971	-0.338865
H	0.518193	-2.057644	-0.616155
C	-1.183709	0.378598	-0.608342
C	-1.326124	1.718832	-0.402185
N	-0.113322	2.268483	-0.006729
H	0.044801	3.245012	0.189606
H	-2.198294	2.347295	-0.517524
C	-2.241028	-0.611729	-0.980724
H	-1.855388	-1.294196	-1.748725
H	-3.099134	-0.088996	-1.421604
C	-2.722359	-1.428646	0.236697
N	-3.337548	-0.653043	1.304400
H	-4.147416	-0.153356	0.941039
H	-2.681742	0.059110	1.621275
H	-1.871921	-1.972347	0.663715
H	-3.443684	-2.180913	-0.099216
H	2.649121	2.324794	0.679452
H	3.985402	0.209564	0.635933

2 site 6

E=-572.2458028 Ha

O	3.222950	-1.965079	0.038222
C	2.356649	-0.910288	0.027541
C	2.843630	0.349845	0.386961
C	2.126010	1.508278	0.431329
C	0.770682	1.384533	0.076545
C	0.211921	0.141638	-0.297287
C	1.018012	-1.012846	-0.319866
H	0.597989	-1.975306	-0.609353
C	-1.176603	0.372115	-0.603951
C	-1.396209	1.707636	-0.398235
N	-0.232939	2.323696	0.008613
H	-0.128090	3.306561	0.201277
H	-2.305504	2.279658	-0.524769
C	-2.181315	-0.668023	-0.991271

H	-1.767398	-1.315565	-1.775841
H	-3.068306	-0.183779	-1.420014
C	-2.616403	-1.532302	0.208837
N	-3.253419	-0.805690	1.299721
H	-4.085565	-0.333651	0.948764
H	-2.623472	-0.067234	1.610662
H	-1.738781	-2.045328	0.619558
H	-3.307581	-2.309866	-0.134357
H	2.568875	2.457256	0.719789
H	2.740488	-2.761678	-0.223454

2 site 7

E=-572.2484642 Ha

O	3.237346	-1.871439	0.006095
C	2.357884	-0.826905	0.013859
C	2.894404	0.427806	0.402834
C	2.058987	1.504419	0.427260
C	0.719207	1.424934	0.091670
C	0.187967	0.169959	-0.296821
C	1.024883	-0.962012	-0.332252
H	0.630465	-1.930909	-0.631409
C	-1.204651	0.380905	-0.595706
C	-1.449050	1.710895	-0.372574
N	-0.301472	2.346661	0.038711
H	-0.209843	3.328265	0.243432
H	-2.370857	2.264519	-0.490174
C	-2.191199	-0.672972	-0.993862
H	-1.768127	-1.300471	-1.789639
H	-3.089061	-0.199240	-1.411676
C	-2.603769	-1.562940	0.195220
N	-3.249327	-0.865344	1.299841
H	-4.090568	-0.401566	0.959802
H	-2.630905	-0.122299	1.622586
H	-1.714405	-2.064998	0.593964
H	-3.281482	-2.348442	-0.156653
H	3.945411	0.486489	0.666104
H	2.768230	-2.673587	-0.262726

2 site 9

E=-572.2801649 Ha

O	3.258079	-1.868148	0.058081
C	2.367814	-0.837001	0.033214
C	2.849019	0.423576	0.393785
C	2.006108	1.540532	0.397278
C	0.683194	1.370424	0.035336
C	0.194845	0.095389	-0.331296
C	1.027841	-1.019340	-0.336158
H	0.662677	-2.005467	-0.618914
C	-1.198647	0.301162	-0.639340
C	-1.408684	1.707130	-0.415772
N	-0.332987	2.348659	-0.025815
H	-2.354845	2.222519	-0.554614
C	-2.212991	-0.726034	-0.980849
H	-1.786295	-1.463890	-1.672462
H	-3.068487	-0.258321	-1.483184
C	-2.719091	-1.462558	0.288958
N	-3.373541	-0.632111	1.284248
H	-4.168799	-0.148292	0.872545
H	-2.734729	0.086750	1.618211
H	-1.870083	-1.961365	0.769257
H	-3.418347	-2.245703	-0.021631
H	2.378782	2.519788	0.678968
H	3.894123	0.508344	0.670668
H	2.810607	-2.684695	-0.203470

2 site 10

E=-572.285088 Ha

O	-3.500719	-1.850292	0.091591
C	-2.560185	-0.859071	0.054289
C	-3.042805	0.458448	0.173000
C	-2.176703	1.536260	0.147105
C	-0.812998	1.274572	-0.000061
C	-0.315668	-0.036344	-0.119369
C	-1.205726	-1.116285	-0.091302
H	-0.844948	-2.138625	-0.183799
C	1.132109	0.049989	-0.259358
C	1.423278	1.417639	-0.211486
N	0.266477	2.137716	-0.057530
H	0.210397	3.142185	-0.007469
H	2.377183	1.920459	-0.284870
C	2.037859	-1.014143	-0.411038
H	1.654922	-2.030306	-0.388602
C	3.519650	-0.794562	-0.442431
N	4.151841	-0.595646	0.878188
H	3.983501	-1.429120	1.440330
H	3.644925	0.147714	1.358584
H	3.757269	0.089423	-1.047767
H	4.023584	-1.639764	-0.920221
H	-2.551883	2.550930	0.238566
H	-4.112020	0.601002	0.284408
H	-3.058258	-2.705069	-0.002582

2 site 11

E=-572.2830242 Ha

O	2.872365	-2.086805	-0.193458
C	2.094126	-0.963688	-0.114285
C	2.758576	0.222212	0.265149
C	2.071323	1.414631	0.383313
C	0.699165	1.408689	0.112241
C	0.021800	0.230793	-0.271980
C	0.737365	-0.974694	-0.381547
H	0.220732	-1.891930	-0.656996
C	-1.362197	0.576979	-0.470660

C	-1.464126	1.913441	-0.193554
N	-0.233166	2.423561	0.150228
H	-0.046303	3.381156	0.399325
H	-2.336792	2.551752	-0.220830
C	-2.462443	-0.356592	-0.891969
H	-2.309277	-0.674268	-1.931243
H	-3.415436	0.200647	-0.875776
C	-2.533159	-1.581481	-0.027069
N	-2.576415	-1.366106	1.353247
H	-1.917665	-0.654046	1.657669
H	-2.469508	-2.206906	1.908614
H	-3.128094	-2.421289	-0.375709
H	2.586320	2.324182	0.677658
H	3.823540	0.167049	0.462543
H	2.318048	-2.825835	-0.479759

2 site 12

20.rad

E=-572.2670346 Ha

O	3.111826	-1.983478	-0.009446
C	2.257126	-0.916703	-0.004140
C	2.825760	0.326234	0.348141
C	2.058778	1.473653	0.384417
C	0.701684	1.364257	0.063902
C	0.117010	0.128920	-0.288271
C	0.915572	-1.028217	-0.321814
H	0.489987	-1.991643	-0.596977
C	-1.274743	0.375943	-0.561354
C	-1.470987	1.717640	-0.360502
N	-0.292203	2.318221	0.011820
H	-0.172290	3.299248	0.205723
H	-2.376899	2.299172	-0.467463
C	-2.299527	-0.649878	-0.931301
H	-1.917176	-1.295787	-1.731432
H	-3.198202	-0.160030	-1.322399
C	-2.706066	-1.539450	0.265694
N	-3.357185	-0.813251	1.324972
H	-2.772017	0.022146	1.479651
H	-1.792646	-2.007008	0.674842
H	-3.362360	-2.348445	-0.071785
H	2.501471	2.427713	0.653868
H	3.883106	0.350490	0.587566
H	2.620485	-2.777222	-0.262211

Table S11. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine radicals obtained with the RAF mechanism (radical ·OH). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

1 site 1

E=-1163.7943994 Ha

F	-5.569950	-0.365733	0.137333
C	-4.626053	-0.074141	-0.767814
F	-4.858477	-0.838022	-1.848542
F	-4.817384	1.197979	-1.152600
C	-3.236723	-0.282466	-0.240814
C	-3.033037	-0.732463	1.022556
C	-1.656091	-0.880510	1.594128
C	-0.585117	-0.714867	0.554850
C	-0.837289	-0.247924	-0.711004
C	-2.158264	-0.011839	-1.124322
H	-2.360833	0.362238	-2.121085
H	-0.021889	-0.053311	-1.397680
O	0.616096	-1.038145	1.061720
C	1.793312	-0.784064	0.293060
C	2.039872	0.702855	0.139287
C	1.564471	1.602881	1.094108
C	1.834475	2.962400	0.960746
C	2.580054	3.429556	-0.119049
C	3.051165	2.532410	-1.074787
C	2.778356	1.172871	-0.949292
H	3.141859	0.459507	-1.686678
H	3.625471	2.892075	-1.923347
H	2.786420	4.490696	-0.219958
H	1.453786	3.660131	1.700363
H	0.958987	1.238499	1.920467
C	2.912899	-1.490893	1.060863
C	4.275405	-1.365557	0.391451
N	4.227337	-1.830482	-0.989427
H	3.952815	-2.811630	-0.997561
C	5.509496	-1.682832	-1.661372
H	5.449828	-2.104420	-2.667752
H	6.349084	-2.160197	-1.128983
H	5.738089	-0.615800	-1.755580
H	5.029260	-1.902017	0.994482
H	4.579646	-0.312184	0.372688
H	2.956107	-1.070070	2.071636
H	2.634403	-2.547726	1.161718
H	1.688540	-1.247022	-0.695929
H	-1.532609	-1.873329	2.056744
H	-3.875165	-0.946961	1.672998
O	-1.390486	0.118841	2.591588
H	-1.979326	-0.051192	3.341700

1 site 2

E=-1163.7861648 Ha

F	-5.315244	-0.932331	-0.599891
C	-4.468003	0.089205	-0.826396
F	-4.501766	0.349117	-2.145545
F	-4.976876	1.161477	-0.208694
C	-3.086439	-0.249723	-0.363161
C	-2.978743	-0.968894	0.946531
C	-1.558401	-1.212318	1.347757
C	-0.485235	-0.843229	0.583003
C	-0.678870	-0.193748	-0.660009
C	-1.997935	0.085878	-1.099523
H	-2.133642	0.589656	-2.051019
H	0.159646	0.126608	-1.263299
O	0.745332	-1.140345	1.093380
C	1.909199	-0.813727	0.340390
C	2.151821	0.681686	0.290505
C	1.726608	1.502718	1.334925
C	1.982720	2.870910	1.298775
C	2.668287	3.427148	0.221746
C	3.095444	2.610189	-0.822904
C	2.835522	1.242812	-0.791165
H	3.168505	0.592049	-1.597533
H	3.626214	3.039592	-1.667343
H	2.864337	4.494546	0.193676
H	1.640759	3.504734	2.111267
H	1.180724	1.065487	2.166209
C	3.046474	-1.561263	1.041569
C	4.401074	-1.361291	0.373852
N	4.348160	-1.717088	-1.039023
H	4.091290	-2.699586	-1.121447
C	5.621059	-1.493758	-1.707637
H	5.559550	-1.837142	-2.743237
H	6.474265	-1.995087	-1.220857
H	5.829276	-0.418493	-1.720519
H	5.169205	-1.930507	0.926804
H	4.688480	-0.304654	0.435167
H	3.093082	-1.221401	2.082423
H	2.783486	-2.626439	1.061309
H	1.810524	-1.201560	-0.681431
H	-1.376231	-1.704065	2.298824
H	-3.489719	-1.943117	0.831207
O	-3.694230	-0.207638	1.923107
H	-3.948203	-0.807066	2.638681

1 site 3

E=-1163.7964435 Ha

F	5.364925	0.018288	-0.388090
C	4.257982	0.420910	0.245901
F	4.617461	0.877700	1.450407
F	3.744192	1.446791	-0.443065
C	3.235649	-0.716254	0.360282
C	2.887385	-1.229739	-1.006867
C	1.608801	-1.347978	-1.433543
C	0.511946	-0.931960	-0.623930
C	0.756428	-0.381378	0.658426
C	2.031067	-0.246295	1.120929
H	2.223876	0.180556	2.099640
H	-0.070137	-0.042006	1.272718
O	-0.707921	-1.123593	-1.172043
C	-1.875375	-0.793136	-0.417937
C	-2.043259	0.704704	-0.266597
C	-1.581320	1.574511	-1.254123
C	-1.774596	2.947156	-1.123327
C	-2.434876	3.458436	-0.008852
C	-2.899646	2.592237	0.978288
C	-2.701947	1.219911	0.852460
H	-3.064933	0.531257	1.612913
H	-3.410763	2.986341	1.851480
H	-2.581956	4.529180	0.092846
H	-1.403871	3.619042	-1.891288
H	-1.056290	1.172198	-2.115993
C	-3.031478	-1.433752	-1.189375
C	-4.385624	-1.212150	-0.527210
N	-4.371633	-1.665753	0.858269
H	-4.175205	-2.665374	0.875203
C	-5.637628	-1.412357	1.529895
H	-5.609335	-1.828420	2.539924
H	-6.512567	-1.827754	1.002716
H	-5.781751	-0.329937	1.614642
H	-5.171784	-1.702438	-1.127995
H	-4.618757	-0.140584	-0.518941
H	-3.042752	-1.019977	-2.204125
H	-2.821283	-2.506958	-1.279866
H	-1.808748	-1.256102	0.573993
H	1.377989	-1.767974	-2.407973
H	3.720216	-1.552551	-1.623197
O	3.955701	-1.705263	1.104996
H	3.347000	-2.449589	1.222023

1 site 4

E=-1163.7932833 Ha

F	5.501733	-0.804158	-0.417039
C	4.622614	-0.106872	0.322863
F	4.897483	-0.353480	1.612547
F	4.883832	1.193508	0.107412
C	3.208226	-0.459131	-0.011072
C	2.900153	-1.106430	-1.171160
C	1.563254	-1.380943	-1.512243
C	0.503222	-0.950743	-0.657582
C	0.765350	-0.306248	0.511621
C	2.163306	-0.034403	0.982721
H	2.341724	-0.580223	1.922839
H	-0.021935	0.069240	1.154811
O	-0.733095	-1.244044	-1.146711

C	-1.871735	-0.878131	-0.372790
C	-2.095057	0.621057	-0.374359
C	-1.739442	1.386320	-1.485128
C	-1.984192	2.756755	-1.499866
C	-2.590322	3.371318	-0.406521
C	-2.949407	2.610055	0.703401
C	-2.700519	1.240126	0.721432
H	-2.983087	0.632925	1.579064
H	-3.417931	3.084846	1.560189
H	-2.778654	4.440409	-0.417998
H	-1.699071	3.346777	-2.365731
H	-1.258123	0.902252	-2.330584
C	-3.040171	-1.637072	-1.006152
C	-4.368880	-1.379651	-0.306380
N	-4.274389	-1.665632	1.119889
H	-4.041275	-2.649629	1.244113
C	-5.514934	-1.371122	1.820890
H	-5.424988	-1.664601	2.869659
H	-6.399457	-1.869909	1.390635
H	-5.691398	-0.290659	1.786819
H	-5.165040	-1.960060	-0.805364
H	-4.638778	-0.321773	-0.410690
H	-3.114461	-1.344384	-2.059796
H	-2.796896	-2.706881	-0.984274
H	-1.737497	-1.225371	0.659270
H	1.306413	-1.894553	-2.430773
H	3.695182	-1.408151	-1.845394
O	2.330802	1.326738	1.369674
H	2.188101	1.865485	0.575968

1 site 5

E=-1163.7968068 Ha

F	5.473132	-0.909789	-0.080259
C	4.661618	0.034618	0.425700
F	4.823097	0.031149	1.754489
F	5.116076	1.212237	-0.032701
C	3.237424	-0.198135	0.014370
C	2.957148	-0.214394	-1.382079
C	1.644786	-0.418367	-1.813903
C	0.619455	-0.604355	-0.913122
C	0.846281	-0.676203	0.575423
C	2.267798	-0.379867	0.943884
H	2.498687	-0.369315	2.003328
H	0.171768	0.019479	1.093475
O	-0.611077	-0.831689	-1.413572
C	-1.761769	-0.659927	-0.570375
C	-1.960332	0.798820	-0.215149
C	-1.577637	1.806588	-1.101529
C	-1.793810	3.143776	-0.777996
C	-2.397587	3.482705	0.430220
C	-2.782579	2.479462	1.317201
C	-2.561336	1.142326	0.999036
H	-2.863188	0.347919	1.678087
H	-3.249493	2.739073	2.262548
H	-2.563619	4.525609	0.681978
H	-1.487201	3.922361	-1.469856
H	-1.099417	1.537957	-2.039449
C	-2.923624	-1.225627	-1.387986
C	-4.262902	-1.113718	-0.670250
N	-4.199469	-1.713761	0.655762
H	-3.955459	-2.698482	0.564304
C	-5.456494	-1.588141	1.376241
H	-5.386184	-2.108887	2.334341
H	-6.327850	-1.980645	0.825464
H	-5.641336	-0.528086	1.581223
H	-5.055111	-1.554901	-1.301145
H	-4.519475	-0.055308	-0.538293
H	-2.971330	-0.692119	-2.344279
H	-2.696559	-2.275254	-1.613487
H	-1.636960	-1.251739	0.340343
H	1.400928	-0.429523	-2.871370
H	3.759364	-0.063611	-2.094935
O	0.449503	-1.960704	1.081854
H	1.061943	-2.608778	0.699272

1 site 6

E=-1163.7943432 Ha

F	5.473876	-0.583098	-0.133649
C	4.507280	0.298829	0.163711
F	4.802113	0.838816	1.356080
F	4.591450	1.287666	-0.742481
C	3.155332	-0.341136	0.163744
C	2.894778	-1.431010	-0.707734
C	1.654686	-1.976141	-0.772967
C	0.502450	-1.497438	0.066171
C	0.874971	-0.335405	0.953019
C	2.129400	0.186654	0.986573
H	2.361487	1.011573	1.652453
H	0.091347	0.058077	1.593203
O	-0.525350	-1.205615	-0.842075
C	-1.746369	-0.709258	-0.289300
C	-1.747310	0.805716	-0.226987
C	-0.979706	1.554893	-1.119856
C	-1.005692	2.946192	-1.072599
C	-1.799900	3.601049	-0.134218
C	-2.567650	2.857676	0.759667
C	-2.540175	1.466111	0.715877
H	-3.140154	0.873522	1.403803
H	-3.185102	3.362611	1.496783
H	-1.816986	4.686029	-0.096551
H	-0.399823	3.520643	-1.766995
H	-0.347751	1.036265	-1.834694
C	-2.845760	-1.256933	-1.204634
C	-4.251004	-0.838162	-0.792828

N	-4.519901	-1.194279	0.594989
H	-4.406621	-2.200760	0.704814
C	-5.858677	-0.807173	1.010138
H	-6.043883	-1.151561	2.030702
H	-6.658383	-1.196021	0.357298
H	-5.927855	0.286085	1.005472
H	-4.983658	-1.279569	-1.492240
H	-4.352483	0.250847	-0.877977
H	-2.644307	-0.918842	-2.227826
H	-2.756315	-2.350454	-1.201845
H	-1.891367	-1.120230	0.715315
H	1.422469	-2.807438	-1.430324
H	3.702800	-1.823014	-1.316908
O	0.013226	-2.570113	0.870043
H	0.645999	-2.709226	1.590645

1 site 8

E=-1163.7906441 Ha

F	5.919826	-0.637458	-0.628922
C	5.164799	-0.145867	0.367670
F	5.357193	-0.926848	1.442851
F	5.673718	1.060844	0.672430
C	3.720246	-0.069629	-0.016477
C	3.366882	0.214683	-1.335309
C	2.031569	0.328423	-1.683032
C	1.033299	0.168460	-0.714393
C	1.385702	-0.099377	0.610740
C	2.729544	-0.221561	0.947202
H	3.007564	-0.432560	1.974738
H	0.626570	-0.164350	1.378534
O	-0.238286	0.287458	-1.177135
C	-1.342373	-0.251796	-0.454337
C	-2.070104	0.899720	0.288941
C	-2.698548	1.856361	-0.683609
C	-3.992589	2.265432	-0.577736
C	-4.834364	1.784360	0.459131
C	-4.327033	0.856830	1.401542
C	-3.048931	0.391039	1.311713
H	-2.659512	-0.327754	2.025653
H	-4.972028	0.506243	2.202628
H	-5.856743	2.136298	0.536244
H	-4.390116	2.982998	-1.289999
H	-2.042419	2.236146	-1.461893
C	-2.178204	-0.972368	-1.512852
C	-3.475935	-1.590553	-1.009503
N	-3.235502	-2.423737	0.161525
H	-2.637490	-3.204155	-0.105441
C	-4.470736	-2.932136	0.735218
H	-4.243850	-3.607931	1.563723
H	-5.112952	-3.464552	0.013622
H	-5.043953	-2.087298	1.133084
H	-3.956829	-2.145172	-1.835177
H	-4.176383	-0.800718	-0.717402
H	-2.397695	-0.266854	-2.321666
H	-1.534423	-1.750198	-1.942674
H	-0.993113	-0.969892	0.295385
H	1.728552	0.531405	-2.704396
H	4.138985	0.328873	-2.089419
O	-1.004654	1.561875	0.997542
H	-1.408104	2.309997	1.463836

1 site 9

E=-1163.7934175 Ha

F	-5.688570	-0.949511	0.071223
C	-4.839054	-0.065084	-0.477072
F	-5.010211	-0.111230	-1.807024
F	-5.244302	1.151496	-0.073408
C	-3.421980	-0.343785	-0.082256
C	-3.139577	-0.722383	1.232580
C	-1.831461	-0.936639	1.624476
C	-0.784805	-0.777595	0.704696
C	-1.064267	-0.395439	-0.609951
C	-2.386994	-0.181828	-0.992449
H	-2.608808	0.110859	-2.013216
H	-0.270324	-0.252611	-1.331713
O	0.454401	-1.024352	1.195213
C	1.587454	-0.879302	0.338510
C	1.842254	0.571229	-0.002267
C	1.596555	1.598453	1.072624
C	1.797126	3.005091	0.594331
C	2.297541	3.299915	-0.634813
C	2.592680	2.270003	-1.566377
C	2.344671	0.921632	-1.225779
H	2.560795	0.133308	-1.944931
H	2.994970	2.517382	-2.542165
H	2.470793	4.334758	-0.915611
H	1.577653	3.788764	1.313496
H	0.581557	1.475830	1.474121
C	2.737785	-1.548465	1.100309
C	4.064040	-1.459047	0.358312
N	3.949504	-1.996092	-0.992287
H	3.686902	-2.978686	-0.931921
C	5.191319	-1.873052	-1.739885
H	5.085344	-2.355664	-2.714606
H	6.065961	-2.306641	-1.226615
H	5.396988	-0.810747	-1.910574
H	4.852928	-1.957728	0.948817
H	4.360676	-0.406411	0.264358
H	2.820301	-1.075129	2.081900
H	2.460878	-2.598715	1.257912
H	1.415254	-1.436186	-0.591459
H	-1.582800	-1.235538	2.636881
H	-3.950268	-0.854365	1.942334
O	2.431235	1.350144	2.219949

H	3.337623	1.554803	1.940626

1 site 10

E=-1163.7901262 Ha

F	-5.768755	-0.784467	-0.713051
C	-4.968529	0.281213	-0.537440
F	-4.986615	0.986088	-1.677763
F	-5.551726	1.036739	0.409114
C	-3.583628	-0.127769	-0.143054
C	-3.413271	-0.873709	1.026556
C	-2.147867	-1.267596	1.416986
C	-1.032184	-0.920862	0.641094
C	-1.198790	-0.171308	-0.524823
C	-2.480630	0.218951	-0.909030
H	-2.615158	0.802136	-1.813427
H	-0.346599	0.125891	-1.122994
O	0.159104	-1.369089	1.110277
C	1.341219	-1.119874	0.351501
C	1.754928	0.336880	0.400857
C	1.553410	1.079630	1.593048
C	2.049854	2.403601	1.691224
C	2.738367	2.974730	0.667223
C	3.031992	2.246062	-0.611795
C	2.410350	0.887474	-0.658720
H	2.590362	0.296166	-1.553656
H	3.117080	3.990379	0.757704
H	1.876271	2.964080	2.605314
H	1.014363	0.627356	2.418391
C	2.411228	-2.021833	0.974633
C	3.784646	-1.834898	0.338713
N	3.723067	-2.011788	-1.107601
H	3.541037	-2.991962	-1.315779
C	4.956195	-1.592058	-1.760374
H	4.895720	-1.806303	-2.830656
H	5.860510	-2.078207	-1.357510
H	5.066495	-0.509367	-1.632550
H	4.511573	-2.510094	0.822743
H	4.134724	-0.812536	0.522713
H	2.468030	-1.802889	2.047433
H	2.074363	-3.061193	0.875412
H	1.181549	-1.420834	-0.690315
H	-1.986863	-1.851461	2.316689
H	-4.278371	-1.144119	1.624828
O	4.444546	2.040621	-0.796482
H	4.862925	2.911363	-0.872343
H	2.661450	2.844810	-1.463452

1 site 11

E=-1163.7904042 Ha

F	5.847770	-0.628280	0.031894
C	4.910377	0.211271	0.501108
F	5.041254	0.259334	1.835780
F	5.225165	1.432813	0.036304
C	3.534300	-0.210277	0.087982
C	3.334892	-0.771007	-1.175083
C	2.059896	-1.117070	-1.584229
C	0.965922	-0.906635	-0.734520
C	1.162011	-0.342231	0.528593
C	2.450475	0.001058	0.929948
H	2.608256	0.435002	1.911754
H	0.328108	-0.155736	1.193982
O	-0.235579	-1.295752	-1.231055
C	-1.397455	-1.163704	-0.411846
C	-1.794712	0.277831	-0.229867
C	-1.606770	1.215755	-1.280646
C	-2.012795	2.505460	-1.153508
C	-2.678744	3.033879	0.084620
C	-2.878183	1.974670	1.123809
C	-2.448009	0.696825	0.963306
H	-2.622800	-0.046942	1.738406
H	-3.400871	2.282241	2.024362
H	-2.040780	3.828665	0.518144
H	-1.858077	3.211271	-1.966711
H	-1.121760	0.879876	-2.193649
C	-2.478139	-1.978129	-1.132121
C	-3.822958	-1.932882	-0.417326
N	-3.691054	-2.352574	0.972800
H	-3.383372	-3.323553	0.996003
C	-4.943069	-2.224651	1.703890
H	-4.819602	-2.613698	2.717603
H	-5.791672	-2.744384	1.228826
H	-5.200325	-1.162587	1.777848
H	-4.558883	-2.536463	-0.977066
H	-4.199972	-0.902806	-0.413648
H	-2.586332	-1.586542	-2.149959
H	-2.120475	-3.011915	-1.219178
H	-1.208692	-1.618521	0.569035
H	1.877517	-1.562321	-2.556223
H	4.183558	-0.943221	-1.829392
O	-3.963585	3.602216	-0.194416
H	-3.823070	4.392135	-0.736442

1 site 12

E=-1163.7929353 Ha

F	5.746795	-0.897701	-0.060345
C	4.881377	-0.028329	0.487637
F	5.014847	-0.110904	1.819844
F	5.296602	1.198152	0.127343
C	3.476549	-0.296165	0.044119
C	3.230884	-0.587799	-1.299503
C	1.935593	-0.795721	-1.736204
C	0.867380	-0.715292	-0.832965
C	1.109332	-0.418106	0.510071
C	2.418514	-0.211758	0.938583

H	2.611851	0.016606	1.981217
H	0.295081	-0.329817	1.219160
O	-0.359058	-0.952472	-1.364621
C	-1.491742	-0.971354	-0.501621
C	-1.859026	0.418592	-0.013815
C	-1.611068	1.514393	-0.782471
C	-1.994057	2.904976	-0.370941
C	-2.690864	2.946268	0.956726
C	-2.922167	1.827966	1.697531
C	-2.502136	0.550627	1.249523
H	-2.696607	-0.341767	1.837256
H	-3.439569	1.907398	2.649567
H	-3.023564	3.923611	1.293837
H	-1.089500	3.531132	-0.327033
H	-1.117076	1.410626	-1.745150
C	-2.607574	-1.607491	-1.332917
C	-3.929268	-1.712477	-0.582559
N	-3.762638	-2.426016	0.677560
H	-3.441943	-3.372685	0.480434
C	-4.999451	-2.483398	1.442088
H	-4.850273	-3.086638	2.340860
H	-5.852929	-2.896112	0.878954
H	-5.266312	-1.468622	1.757133
H	-4.688008	-2.176184	-1.237306
H	-4.296109	-0.706689	-0.341926
H	-2.743159	-1.008115	-2.240314
H	-2.268086	-2.601583	-1.649617
H	-1.280780	-1.613116	0.363318
H	1.716782	-1.031413	-2.771973
H	4.059872	-0.658981	-1.996835
O	-2.777932	3.545257	-1.384389
H	-3.593129	3.026659	-1.463685

1 site 13

E=-1163.7966778 Ha

F	-5.583139	-1.168070	-0.673145
C	-4.882899	-0.030783	-0.520814
F	-4.958432	0.640804	-1.678587
F	-5.534979	0.691034	0.406298
C	-3.467979	-0.301675	-0.113200
C	-3.230186	-0.916266	1.119094
C	-1.935393	-1.187261	1.518553
C	-0.857460	-0.847357	0.688703
C	-1.093074	-0.231000	-0.540015
C	-2.402634	0.036405	-0.934353
H	-2.588736	0.518004	-1.887997
H	-0.274460	0.046834	-1.191488
O	0.366793	-1.174936	1.170968
C	1.540543	-0.833443	0.426773
C	1.778069	0.662304	0.410572
C	1.519171	1.403402	1.529118
C	1.689644	2.804272	1.551566
C	2.150834	3.475155	0.388945
C	2.420941	2.788980	-0.750304
C	2.248703	1.305746	-0.875276
H	1.468290	1.119225	-1.645056
H	2.803655	3.289166	-1.634607
H	2.298447	4.550618	0.419898
H	1.473515	3.362249	2.455247
H	1.148663	0.898007	2.418382
C	2.641808	-1.628493	1.139230
C	4.032447	-1.471007	0.543484
N	4.047382	-1.853883	-0.868968
H	3.688387	-2.802591	-0.964116
C	5.388664	-1.774215	-1.442146
H	5.368067	-2.127233	-2.475619
H	6.133774	-2.357764	-0.880318
H	5.701003	-0.725495	-1.444632
H	4.750827	-2.060695	1.136205
H	4.345115	-0.421789	0.594072
H	2.657968	-1.305636	2.186120
H	2.344053	-2.684856	1.134614
H	1.433777	-1.203775	-0.604449
H	-1.722374	-1.663421	2.469386
H	-4.065722	-1.177593	1.761701
O	3.475944	0.788646	-1.374807
H	3.403936	-0.188234	-1.464512

Table S12. Cartesian Coordinates (in Å) and electronic energies (in Ha) for serotonine and serotonine radicals obtained with the RAF mechanism (radical ·OH and ·OCH3). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

2 RAF 1

E=-648.71141 Ha

O	3.624898	-1.594292	-0.379436
C	2.606311	-0.712665	-0.153103
C	2.972196	0.525983	0.407570
C	2.013239	1.497345	0.691120
C	0.686846	1.224169	0.396434
C	0.303685	-0.018108	-0.189984
C	1.285981	-0.999363	-0.451988
H	1.009981	-1.953390	-0.896493
C	-1.079375	0.015963	-0.403278
C	-1.582506	1.384837	-0.018190
N	-0.447594	1.991737	0.646064
H	-0.382590	2.997484	0.544200
H	-2.454456	1.335465	0.656081
C	-1.958182	-1.083384	-0.891875
H	-1.519076	-1.560312	-1.779457
H	-2.931482	-0.677884	-1.205230
C	-2.198508	-2.161728	0.190422
N	-2.784378	-1.685407	1.435178
H	-3.670213	-1.218341	1.250013
H	-2.169518	-0.990751	1.856039
H	-1.239729	-2.632234	0.435626
H	-2.845236	-2.946078	-0.217879
H	2.303730	2.442931	1.137652
H	4.021674	0.698169	0.618896
H	3.259420	-2.403536	-0.762710
O	-1.918417	2.205976	-1.135019
H	-2.708674	1.832392	-1.552554

2 RAF 2

E=-648.7014016 Ha

O	-3.641362	-1.172429	-0.514949
C	-2.533195	-0.425980	-0.235267
C	-2.668811	0.963829	-0.316291
C	-1.594833	1.804649	-0.041439
C	-0.383359	1.223567	0.316691
C	-0.242180	-0.160997	0.398636
C	-1.311482	-0.998912	0.124439
H	-1.200203	-2.078554	0.208735
C	1.179257	-0.512175	0.808909
C	1.725299	0.864876	1.101637
N	0.844789	1.834636	0.629355
H	0.873825	2.785063	0.974471
H	2.774643	1.102164	1.224567
C	1.936158	-1.301709	-0.273797
H	1.512985	-2.315018	-0.278084
H	2.978015	-1.399579	0.059732
C	1.886935	-0.728670	-1.694554
N	2.521782	0.567238	-1.921418
H	3.469892	0.552503	-1.549159
H	2.023706	1.289821	-1.406640
H	0.843933	-0.646849	-2.020724
H	2.361767	-1.454613	-2.364621
H	-1.709424	2.882312	-0.106293
H	-3.635085	1.368319	-0.597332
H	-3.418882	-2.110113	-0.433470
O	1.230597	-1.366444	1.952984
H	0.882215	-0.848469	2.695197

2 RAF 3

E=-648.6745788 Ha

O	-2.841108	-2.225226	-0.313437
C	-2.112290	-1.078718	-0.171082
C	-2.804757	0.106050	-0.607370
C	-2.134281	1.321787	-0.683415
C	-0.826480	1.372997	-0.233575
C	-0.208988	0.274095	0.604803
C	-0.842425	-1.047288	0.309140
H	-0.346621	-1.950278	0.658230
C	1.276377	0.505131	0.371188
C	1.407481	1.704075	-0.213051
N	0.153991	2.290477	-0.493512
H	0.041383	3.013094	-1.189772
H	2.310645	2.257613	-0.438204
C	2.336834	-0.415486	0.877985
H	1.991594	-0.869057	1.816029
H	3.246752	0.150893	1.114849
C	2.697019	-1.514521	-0.143954
N	3.255462	-1.031499	-1.400466
H	4.107846	-0.506172	-1.211214
H	2.600715	-0.367938	-1.812527
H	1.802115	-2.099484	-0.383341
H	3.417623	-2.204653	0.308016
H	-2.598735	2.181003	-1.158670
H	-3.825395	-0.004862	-0.953225
H	-2.312577	-2.969950	0.006878
O	-0.375582	0.578566	2.015330
H	-1.298936	0.361486	2.221635

2 RAF 4

E=-648.7131166 Ha

O	-3.230658	-1.572254	-0.372609
C	-2.361531	-0.538134	-0.310093
C	-2.786987	0.754759	-0.493911
C	-1.901175	1.839085	-0.367748

C	-0.564979	1.540312	0.002694
C	-0.072821	0.248874	0.187522
C	-0.930734	-0.944340	-0.054602
H	-0.576937	-1.530041	-0.919348
C	1.293581	0.342460	0.572785
C	1.591204	1.690013	0.607976
N	0.470733	2.404497	0.261566
H	0.405053	3.410065	0.235029
H	2.512145	2.189915	0.873011
C	2.238953	-0.795870	0.817730
H	1.735085	-1.575551	1.400064
H	3.095818	-0.445770	1.408019
C	2.757058	-1.407546	-0.498298
N	3.490093	-0.495568	-1.368241
H	4.304434	-0.139097	-0.869967
H	2.903558	0.316186	-1.558683
H	1.908217	-1.805210	-1.067111
H	3.407111	-2.259188	-0.270575
H	-2.239286	2.859453	-0.504873
H	-3.837914	0.920463	-0.706592
H	-2.785482	-2.328242	0.051042
O	-0.904817	-1.918791	1.005510
H	-1.049190	-1.424808	1.829174

2 RAF 5

E=-648.6976807 Ha

O	-3.059397	-1.119202	1.062773
C	-2.222368	-0.709311	-0.004350
C	-2.599503	0.689726	-0.443543
C	-1.737251	1.728067	-0.492917
C	-0.377501	1.501212	-0.113280
C	0.093047	0.233748	0.309494
C	-0.771802	-0.847458	0.370028
H	-0.460424	-1.835720	0.695447
C	1.502795	0.389879	0.613724
C	1.808805	1.696669	0.359940
N	0.676543	2.367141	-0.074325
H	0.635806	3.346751	-0.308814
H	2.749004	2.219856	0.466025
C	2.430398	-0.705049	1.035402
H	1.966185	-1.299017	1.833432
H	3.349881	-0.274619	1.452363
C	2.798369	-1.631145	-0.141969
N	3.498087	-0.985827	-1.245307
H	4.372315	-0.588572	-0.904624
H	2.940506	-0.197657	-1.571707
H	1.882233	-2.080601	-0.542265
H	3.421922	-2.453429	0.224570
H	-2.060918	2.714646	-0.814308
H	-3.643157	0.800105	-0.721464
H	-2.848992	-0.543982	1.812288
O	-2.576040	-1.641659	-1.009759
H	-1.993207	-1.468101	-1.762811

2 RAF 6

E=-648.700126 Ha

O	2.800326	-2.020473	-0.343625
C	1.924722	-0.974257	-0.317353
C	2.666962	0.303996	-0.005119
C	1.773579	1.498837	0.090517
C	0.427067	1.357703	-0.125452
C	-0.205039	0.118808	-0.443420
C	0.596875	-1.070344	-0.528415
H	0.135318	-2.030878	-0.751002
C	-1.590381	0.360074	-0.604866
C	-1.783463	1.711784	-0.376945
N	-0.579630	2.309333	-0.095853
H	-0.442302	3.287885	0.098838
H	-2.696630	2.289604	-0.413671
C	-2.651428	-0.661429	-0.879579
H	-2.328058	-1.331084	-1.687309
H	-3.563164	-0.162070	-1.232381
C	-2.991263	-1.495539	0.371397
N	-3.492934	-0.736581	1.509565
H	-4.334814	-0.232615	1.234491
H	-2.807241	-0.023641	1.755156
H	-2.092655	-2.030964	0.699942
H	-3.736760	-2.254805	0.110333
H	2.233589	2.446349	0.348515
H	3.404915	0.451350	-0.817335
H	2.311844	-2.846746	-0.471760
O	3.385841	0.165861	1.220961
H	3.928782	-0.632550	1.126933

2 RAF 7

E=-648.699858 Ha

O	-2.496355	2.683594	0.065737
C	-1.889009	1.463656	-0.064946
C	-2.668113	0.352921	0.096664
C	-2.159716	-1.051439	-0.057816
C	-0.695153	-1.030173	-0.308833
C	0.088643	0.106009	-0.470993
C	-0.503487	1.391373	-0.370058
H	0.080763	2.297587	-0.506156
C	1.439969	-0.338635	-0.693927
C	1.407804	-1.708985	-0.633242
N	0.108820	-2.118897	-0.413806
H	-0.195611	-3.066117	-0.245237
H	2.206701	-2.428352	-0.743839
C	2.643281	0.536572	-0.860578
H	2.434997	1.330118	-1.590416
H	3.475690	-0.052903	-1.266096
C	3.084567	1.172199	0.473287
N	3.457353	0.229817	1.519727

H	4.224615	-0.354079	1.189981
H	2.674956	-0.402565	1.683528
H	2.268524	1.793281	0.861504
H	3.934645	1.839581	0.293631
H	-2.673632	-1.527339	-0.914982
H	-3.724944	0.491381	0.306359
H	-1.827809	3.377185	-0.012726
O	-2.379878	-1.882576	1.090209
H	-3.324953	-1.843353	1.298089

2 RAF 8

E=-648.6863036 Ha

O	2.711407	-2.466998	-0.074914
C	1.996973	-1.316386	0.005475
C	2.572406	-0.291949	0.835130
C	2.000069	0.925597	0.940450
C	0.860999	1.271630	0.034332
C	0.087500	0.054848	-0.422840
C	0.736233	-1.163484	-0.565087
H	0.230825	-2.019338	-1.010339
C	-1.284060	0.441858	-0.544447
C	-1.397765	1.666207	0.061096
N	-0.198830	2.108375	0.609416
H	-0.002407	3.102889	0.567545
H	-2.302437	2.248064	0.198900
C	-2.405932	-0.426390	-1.024335
H	-2.113213	-0.941612	-1.948461
H	-3.275393	0.196681	-1.271710
C	-2.828960	-1.470113	0.031532
N	-3.298221	-0.925312	1.297377
H	-4.087679	-0.303218	1.130589
H	-2.563857	-0.348992	1.705515
H	-1.980319	-2.128295	0.249052
H	-3.622054	-2.100400	-0.385645
H	2.400281	1.695970	1.590939
H	3.460362	-0.557830	1.399792
H	2.229912	-3.102590	-0.623955
O	1.449670	1.954235	-1.082576
H	0.791938	1.928424	-1.797696

Table S12. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine reactant complexes obtained with the HAT mechanism (radical ·OH and ·OCH3). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

1 site 7 OH

E=-1163.7635748 Ha

F	-5.282309	-1.259035	-0.787842
C	-4.751725	-0.064063	-0.477472
F	-4.844034	0.700985	-1.574609
F	-5.545062	0.474299	0.462237
C	-3.337403	-0.189538	0.001897
C	-3.093037	-0.553899	1.327472
C	-1.792950	-0.721449	1.769021
C	-0.722747	-0.524850	0.887611
C	-0.960884	-0.153896	-0.438780
C	-2.275797	0.007805	-0.870786
H	-2.468687	0.303023	-1.896609
H	-0.143880	0.021886	-1.128006
O	0.509978	-0.742440	1.422134
C	1.665309	-0.547004	0.635071
C	1.888184	0.898248	0.264491
C	1.437082	1.910784	1.114578
C	1.671279	3.245125	0.796587
C	2.352223	3.576018	-0.372501
C	2.798572	2.567432	-1.223661
C	2.566866	1.230947	-0.911041
H	2.914730	0.428851	-1.557303
H	3.324472	2.822095	-2.138772
H	2.530500	4.617595	-0.621433
H	1.317727	4.027455	1.461158
H	0.899205	1.647863	2.021082
C	2.803191	-1.208043	1.405736
C	4.153976	-1.126219	0.706367
N	4.063291	-1.584403	-0.668658
H	3.535555	-2.453077	-0.723539
C	5.362288	-1.718527	-1.300329
H	5.240019	-2.105631	-2.314694
H	6.058410	-2.377614	-0.753470
H	5.829532	-0.729808	-1.370964
H	4.890316	-1.697424	1.301093
H	4.501712	-0.084466	0.691419
H	2.865699	-0.734977	2.393388
H	2.520117	-2.255925	1.561729
H	1.547003	-1.175028	-0.348447
H	-1.572644	-1.004653	2.792477
H	-3.924366	-0.699039	2.009935
O	1.221233	-2.266128	-1.238940
H	0.297941	-2.411222	-0.947627

1 site 14 OH

E=-1163.7625885 Ha

F	5.230975	-1.161120	1.159915

C	4.788496	-0.059497	0.530603
F	4.947926	0.964305	1.382714
F	5.611820	0.145548	-0.509654
C	3.364005	-0.201650	0.088097
C	3.077364	-0.806587	-1.136232
C	1.761737	-0.986629	-1.526233
C	0.719737	-0.564548	-0.692738
C	1.001393	0.047800	0.529934
C	2.328880	0.222046	0.911769
H	2.555714	0.704554	1.856651
H	0.207138	0.407635	1.172077
O	-0.535173	-0.807431	-1.166252
C	-1.658122	-0.441057	-0.363843
C	-1.847021	1.058136	-0.272096
C	-1.415033	1.899766	-1.296684
C	-1.635420	3.271745	-1.211120
C	-2.294016	3.807819	-0.107144
C	-2.731104	2.967931	0.915066
C	-2.506574	1.596488	0.835501
H	-2.845034	0.926310	1.623996
H	-3.242163	3.382219	1.778746
H	-2.463247	4.878073	-0.041695
H	-1.289193	3.923848	-2.007058
H	-0.894672	1.476777	-2.151455
C	-2.855869	-1.101432	-1.028915
C	-4.134965	-1.065577	-0.218737
N	-3.887882	-1.553081	1.129362
H	-3.442731	-2.468550	1.057571
C	-5.108667	-1.645383	1.913291
H	-4.883781	-2.070809	2.894117
H	-5.896080	-2.254280	1.438729
H	-5.512663	-0.638886	2.067457
H	-4.912425	-1.641756	-0.750909
H	-4.500461	-0.030303	-0.151056
H	-2.982812	-0.757038	-2.060100
H	-2.566214	-2.259809	-1.104977
H	-1.541678	-0.864537	0.640600
H	1.510644	-1.449828	-2.474524
H	3.887086	-1.127853	-1.783248
O	-1.983311	-3.406072	-0.660406
H	-1.069804	-3.090983	-0.817078

1 site 15 OH

E=-1163.7647506 Ha

F	5.502162	-1.367544	1.071622
C	5.057216	-0.264864	0.444649
F	5.267993	0.766324	1.276880
F	5.848510	-0.089691	-0.626265
C	3.616763	-0.384828	0.053150
C	3.276912	-1.063478	-1.118827
C	1.947194	-1.223799	-1.463713
C	0.939834	-0.707111	-0.638901
C	1.276278	-0.020733	0.530017
C	2.618519	0.131864	0.868324
H	2.885883	0.671151	1.770906
H	0.512373	0.414390	1.162421
O	-0.329595	-0.930156	-1.067734
C	-1.419682	-0.515680	-0.250516
C	-1.589692	0.990339	-0.250336
C	-1.233493	1.742304	-1.369592
C	-1.430431	3.120633	-1.378595
C	-1.988936	3.755725	-0.272035
C	-2.347930	3.007700	0.847054
C	-2.146321	1.630139	0.859819
H	-2.428044	1.034866	1.726236
H	-2.779096	3.498402	1.714440
H	-2.139159	4.830834	-0.279591
H	-1.143024	3.700517	-2.250311
H	-0.788109	1.243062	-2.225565
C	-2.640223	-1.234499	-0.835632
C	-3.923423	-0.926684	-0.082411
N	-3.835342	-1.245416	1.312247
H	-3.588883	-2.227369	1.423343
C	-5.062001	-0.952874	2.038287
H	-4.964274	-1.279416	3.075842
H	-5.936637	-1.442720	1.583913
H	-5.225224	0.130105	2.035685
H	-4.768611	-1.533653	-0.576998
H	-4.203358	0.128663	-0.187523
H	-2.748478	-0.939472	-1.884858
H	-2.442188	-2.312858	-0.819964
H	-1.260687	-0.866158	0.777593
H	1.654498	-1.747127	-2.367446
H	4.058520	-1.458914	-1.759715
O	-5.979727	-2.516849	-0.746814
H	-6.645015	-1.837053	-0.972317

1 site 16 OH

E=-1163.7678665 Ha

F	-5.696567	-1.243771	-0.015927
C	-4.924468	-0.266483	-0.518098
F	-5.047118	-0.299622	-1.854127
F	-5.463377	0.895030	-0.108595
C	-3.498715	-0.408563	-0.083065
C	-3.210366	-0.895785	1.193068
C	-1.897523	-0.980117	1.620283
C	-0.855526	-0.577125	0.775494
C	-1.140843	-0.085389	-0.500432
C	-2.466065	-0.006728	-0.920098
H	-2.692619	0.370538	-1.911826
H	-0.350488	0.250115	-1.160292
O	0.392937	-0.714125	1.291611
C	1.519044	-0.407760	0.475112
C	1.669412	1.084492	0.256017

C	1.284737	1.985661	1.248806
C	1.467059	3.353239	1.062691
C	2.039467	3.830076	-0.114226
C	2.426151	2.933833	-1.107973
C	2.238754	1.566249	-0.924881
H	2.539468	0.858255	-1.695017
H	2.866639	3.300383	-2.030285
H	2.178327	4.896952	-0.258940
H	1.157437	4.048798	1.836713
H	0.828229	1.608594	2.159745
C	2.713104	-1.006868	1.223508
C	4.044102	-0.760065	0.529601
N	4.023331	-1.258705	-0.836439
H	3.674000	-2.260279	-0.880315
C	5.276001	-1.084047	-1.543493
H	5.234527	-1.607633	-2.500581
H	6.150813	-1.440544	-0.975276
H	5.426076	-0.015712	-1.737188
H	4.854912	-1.221572	1.115769
H	4.257121	0.315910	0.478990
H	2.740066	-0.571436	2.228719
H	2.553037	-2.085342	1.326717
H	1.412394	-0.911337	-0.494762
H	-1.644102	-1.364945	2.602055
H	-4.017452	-1.217765	1.843254
O	4.034130	-3.581471	-0.292931
H	5.009365	-3.589732	-0.307894

1 site 17 OH

E=-1163.7618508 Ha

F	-5.818536	0.419860	0.335237
C	-4.972896	0.123228	-0.665078
F	-5.500153	-0.931656	-1.310174
F	-4.986856	1.151838	-1.526059
C	-3.593908	-0.163894	-0.156245
C	-3.434863	-0.858554	1.044429
C	-2.166728	-1.174915	1.496907
C	-1.041081	-0.800501	0.752225
C	-1.195904	-0.097507	-0.444552
C	-2.477896	0.212787	-0.891397
H	-2.603569	0.765218	-1.816551
H	-0.336790	0.230172	-1.016764
O	0.153479	-1.172381	1.282787
C	1.345757	-0.914776	0.547519
C	1.709499	0.555889	0.547305
C	1.375492	1.371398	1.628286
C	1.753664	2.711857	1.636391
C	2.473408	3.244445	0.569274
C	2.813014	2.431391	-0.510343
C	2.427666	1.092351	-0.523621
H	2.701779	0.455780	-1.362640
H	3.372120	2.832022	-1.351657
H	2.764672	4.290173	0.577080
H	1.482611	3.342725	2.477396
H	0.805996	0.954144	2.454121
C	2.413357	-1.776516	1.228376
C	3.791056	-1.652027	0.591106
N	3.744738	-1.938405	-0.832457
H	3.334339	-2.847023	-1.027888
C	4.971762	-1.725588	-1.527528
H	5.089204	-0.586296	-1.791606
H	4.975290	-2.235744	-2.491922
H	5.878799	-1.972352	-0.955032
H	4.506244	-2.299484	1.126173
H	4.155071	-0.622573	0.702240
H	2.470757	-1.486758	2.283511
H	2.072952	-2.819174	1.198766
H	1.216822	-1.256389	-0.487614
H	-2.014054	-1.714513	2.425248
H	-4.307814	-1.144128	1.622745
O	5.203163	0.844185	-1.928034
H	4.970775	1.073828	-1.005795

1 site 7 CH3OH

E=-1203.0598865 Ha

F	-5.530556	0.578162	0.496401
C	-4.754099	0.009331	-0.439123
F	-5.312346	-1.177013	-0.734098
F	-4.835560	0.761226	-1.546964
C	-3.338863	-0.140449	0.030688
C	-3.077192	-0.364405	1.381316
C	-1.772620	-0.554253	1.808882
C	-0.726420	-0.522967	0.884577
C	-0.980480	-0.301585	-0.470771
C	-2.293760	-0.112910	-0.887077
H	-2.503415	0.064111	-1.936759
H	-0.172944	-0.293526	-1.194090
O	0.518087	-0.752092	1.403813
C	1.661973	-0.431228	0.652661
C	1.721899	1.016112	0.239699
C	1.178572	1.992230	1.080452
C	1.258371	3.337049	0.734258
C	1.876606	3.716173	-0.455015
C	2.414867	2.745086	-1.296087
C	2.337832	1.397605	-0.954844
H	2.765543	0.628836	-1.591836
H	2.892417	3.036637	-2.226535
H	1.934743	4.765653	-0.726854
H	0.834216	4.089081	1.392423
H	0.689760	1.691840	2.003322
C	2.850472	-0.946639	1.454050
C	4.206384	-0.649092	0.826102
N	4.257488	-1.069420	-0.561620
H	3.824420	-1.981601	-0.684696

C	5.598443	-1.032303	-1.110897
H	5.584787	-1.396180	-2.141123
H	6.332016	-1.626004	-0.538145
H	5.952199	0.004813	-1.125032
H	4.986439	-1.127633	1.446872
H	4.397351	0.432243	0.859182
H	2.801967	-0.499945	2.455343
H	2.721816	-2.029622	1.581306
H	1.643842	-1.134799	-0.351589
H	-1.537236	-0.725820	2.853674
H	-3.893823	-0.379293	2.095565
O	1.587012	-2.174873	-1.184926
C	0.762234	-3.129349	-0.586193
H	1.023443	-4.099615	-1.031926
H	0.946189	-3.211432	0.496266
H	-0.306074	-2.937871	-0.749248

1 site 14 CH3OH

E=-1203.0572063 Ha

F	5.592668	-1.005337	0.260182
C	4.862060	0.086506	0.540237
F	4.979386	0.326039	1.854574
F	5.449526	1.111961	-0.099146
C	3.433109	-0.086675	0.125570
C	3.147135	-0.704198	-1.093937
C	1.835150	-0.834258	-1.511864
C	0.793063	-0.345764	-0.713044
C	1.074982	0.277752	0.504133
C	2.400464	0.401214	0.914734
H	2.626251	0.882684	1.860139
H	0.282275	0.684443	1.120335
O	-0.457101	-0.540263	-1.208138
C	-1.574977	-0.252643	-0.373468
C	-1.857084	1.235464	-0.286268
C	-1.493272	2.090212	-1.326202
C	-1.788843	3.448725	-1.247547
C	-2.454436	3.957494	-0.135178
C	-2.822943	3.103768	0.902740
C	-2.524129	1.746343	0.830199
H	-2.810813	1.065063	1.629222
H	-3.338813	3.497057	1.773424
H	-2.682493	5.017136	-0.075181
H	-1.495764	4.111524	-2.055944
H	-0.966432	1.688199	-2.186702
C	-2.737884	-1.004846	-0.990329
C	-4.035074	-0.957907	-0.216055
N	-3.807525	-1.349734	1.167553
H	-3.402753	-2.286342	1.156123
C	-5.035139	-1.342825	1.946771
H	-4.832024	-1.711771	2.954971
H	-5.843488	-1.950895	1.507632
H	-5.400380	-0.313377	2.031981
H	-4.783088	-1.590495	-0.725754
H	-4.431995	0.068424	-0.222724
H	-2.844313	-0.792917	-2.058260
H	-2.410145	-2.218076	-0.927188
H	-1.398069	-0.648716	0.634733
H	1.583164	-1.315694	-2.450830
H	3.955971	-1.090562	-1.706231
O	-2.155951	-3.371613	-0.461872
C	-0.767423	-3.443560	-0.290960
H	-0.388997	-2.741132	0.466061
H	-0.567842	-4.461407	0.070598
H	-0.215939	-3.292782	-1.226865

1 site 15 CH3OH

E=-1203.0616858 Ha

F	6.071056	-1.426351	0.122287
C	5.383135	-0.291791	0.332339
F	5.606024	0.087526	1.599458
F	5.938779	0.641231	-0.459595
C	3.924091	-0.471592	0.046905
C	3.534657	-1.195063	-1.082540
C	2.192749	-1.334294	-1.385305
C	1.222234	-0.751030	-0.560179
C	1.607916	-0.023070	0.567007
C	2.962861	0.109669	0.862136
H	3.268085	0.672396	1.737775
H	0.872974	0.454818	1.202897
O	-0.064230	-0.962205	-0.943085
C	-1.119785	-0.487989	-0.114245
C	-1.256202	1.020124	-0.170769
C	-0.907065	1.719342	-1.325870
C	-1.073227	3.100446	-1.384996
C	-1.593625	3.790842	-0.293142
C	-1.945849	3.095502	0.861517
C	-1.774974	1.715231	0.924244
H	-2.051826	1.161772	1.819628
H	-2.347785	3.629430	1.717271
H	-1.719932	4.868007	-0.339915
H	-0.791608	3.639112	-2.284587
H	-0.491807	1.176979	-2.170627
C	-2.374693	-1.201471	-0.633116
C	-3.621953	-0.843417	0.151057
N	-3.518594	-1.131135	1.542514
H	-3.229075	-2.096189	1.687942
C	-4.733561	-0.836055	2.289535
H	-4.598351	-1.111021	3.337645
H	-5.606760	-1.363228	1.879173
H	-4.922512	0.241643	2.240129
H	-4.542318	-1.447261	-0.316948
H	-3.906184	0.208672	0.016890
H	-2.514630	-0.938318	-1.686911
H	-2.193775	-2.282199	-0.588915

H	-0.938236	-0.800128	0.922999
H	1.861475	-1.898086	-2.250540
H	4.287399	-1.654694	-1.715447
O	-5.807062	-1.995219	-0.615628
C	-6.577123	-0.905516	-1.006447
H	-6.186949	-0.397287	-1.900619
H	-7.571243	-1.303406	-1.259991
H	-6.716704	-0.164527	-0.203871

1 site 16 CH3OH

E=-1203.0661932 Ha

F	5.237660	-0.478768	1.835888
C	5.102876	-0.520404	0.501632
F	5.753424	0.549053	0.011470
F	5.764412	-1.603042	0.061084
C	3.665345	-0.543211	0.083074
C	3.325938	-1.024507	-1.182920
C	2.007328	-1.004096	-1.599377
C	1.010487	-0.501305	-0.753408
C	1.346993	-0.015794	0.511972
C	2.677883	-0.042563	0.920853
H	2.944003	0.329690	1.904459
H	0.593619	0.394666	1.172678
O	-0.249828	-0.539637	-1.258479
C	-1.337209	-0.118875	-0.440772
C	-1.354530	1.385078	-0.253157
C	-0.903739	2.227528	-1.269516
C	-0.963591	3.609456	-1.112344
C	-1.478814	4.159653	0.059008
C	-1.930747	3.322321	1.076313
C	-1.865688	1.939918	0.922256
H	-2.217499	1.278180	1.711558
H	-2.326833	3.745676	1.994381
H	-1.522391	5.237429	0.181162
H	-0.602986	4.258368	-1.904588
H	-0.491738	1.792402	-2.175795
C	-2.585081	-0.626469	-1.168780
C	-3.882124	-0.249497	-0.466622
N	-3.885996	-0.721712	0.903852
H	-3.637387	-1.829564	0.922764
H	-4.745025	-0.647145	-1.031188
H	-4.006455	0.842475	-0.441642
H	-2.582982	-0.216442	-2.184816
H	-2.508173	-1.717471	-1.242657
H	-1.271333	-0.612665	0.537488
H	1.713933	-1.380846	-2.573124
H	4.097728	-1.423496	-1.833484
O	-3.830943	-3.084956	0.656526
C	-4.809068	-3.300608	-0.297894
H	-4.516699	-2.972820	-1.308729
H	-4.984866	-4.385795	-0.340936
H	-5.775727	-2.836629	-0.035534
C	-5.142416	-0.491033	1.581435
H	-6.011763	-0.843904	1.001692
H	-5.133516	-0.989990	2.551783
H	-5.268302	0.587887	1.736697

1 site 17 CH3OH

E=-1203.058357 Ha

F	-6.101783	-0.679768	-0.669540
C	-5.198551	0.313112	-0.730563
F	-5.174580	0.760443	-1.994817
F	-5.680585	1.311695	0.029191
C	-3.848776	-0.141245	-0.268051
C	-3.754711	-0.964361	0.856226
C	-2.513832	-1.356600	1.323507
C	-1.349895	-0.930260	0.670464
C	-1.439845	-0.102907	-0.450858
C	-2.695535	0.284980	-0.912511
H	-2.771044	0.926070	-1.784256
H	-0.550700	0.257249	-0.953542
O	-0.187295	-1.386861	1.204710
C	1.040688	-1.077844	0.552196
C	1.428893	0.376911	0.718095
C	1.034482	1.096566	1.846475
C	1.433903	2.421139	2.003824
C	2.234596	3.032047	1.040555
C	2.634457	2.313302	-0.083616
C	2.228592	0.991608	-0.246983
H	2.555037	0.436006	-1.122907
H	3.260491	2.768368	-0.845667
H	2.542056	4.065796	1.165867
H	1.115909	2.978979	2.879420
H	0.402398	0.619079	2.590094
C	2.063014	-2.027528	1.183448
C	3.465862	-1.875752	0.610050
N	3.472589	-2.055901	-0.830803
H	3.039849	-2.920283	-1.137370
C	4.665269	-1.718219	-1.510066
H	4.670060	-0.542703	-1.794900
H	4.754766	-2.236308	-2.465686
H	5.582389	-1.832291	-0.911197
H	4.149671	-2.577560	1.116141
H	3.837793	-0.864399	0.810178
H	2.088631	-1.840942	2.262795
H	1.702605	-3.054379	1.042195
H	0.951669	-1.309484	-0.517438
H	-2.411474	-2.002190	2.188973
H	-4.657685	-1.301765	1.355480
O	4.852496	0.808891	-1.979290
C	5.712040	1.186527	-0.952758
H	5.251577	1.124598	0.045209
H	6.655777	0.619845	-0.957766
H	5.969126	2.241193	-1.133455

Table S13. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine metabolites reactant complexes obtained with the HAT mechanism (radical ·OH and ·OCH3). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

M1 site 16 OH

E=-1124.4686 Ha

F	-5.439856	-1.171534	0.003071
C	-4.681737	-0.137743	-0.398063
F	-4.857745	0.003587	-1.720559
F	-5.197055	0.959504	0.183252
C	-3.241682	-0.338127	-0.040436
C	-2.915094	-0.895968	1.197526
C	-1.589180	-1.043055	1.561197
C	-0.571312	-0.633744	0.689741
C	-0.894537	-0.072471	-0.547407
C	-2.233571	0.069927	-0.903102
H	-2.489648	0.502813	-1.864241
H	-0.122383	0.268519	-1.225697
O	0.692683	-0.835419	1.142655
C	1.792593	-0.525477	0.292020
C	1.981803	0.970054	0.135529
C	1.668644	1.835013	1.184322
C	1.883936	3.203852	1.051600
C	2.418108	3.718047	-0.127730
C	2.733609	2.858048	-1.176888
C	2.512958	1.489259	-1.046984
H	2.758053	0.809736	-1.861046
H	3.144539	3.253964	-2.100676
H	2.582671	4.786115	-0.230707
H	1.629943	3.871482	1.869240
H	1.241028	1.429366	2.097020
C	2.996261	-1.195442	0.959712
C	4.302050	-0.990573	0.205701
N	4.172563	-1.453641	-1.172888
H	3.826789	-2.492452	-1.204468
H	5.109248	-1.506197	0.742393
H	4.560253	0.075365	0.169082
H	3.094193	-0.792594	1.974125
H	2.792006	-2.268392	1.042701
H	1.629066	-0.979658	-0.694237
H	-1.306676	-1.482397	2.511652
H	-3.704112	-1.222402	1.867740
O	4.115990	-3.754337	-0.710055
H	4.985330	-3.966815	-1.096657
H	5.067190	-1.386528	-1.659106

M1 site 14 OH

E=-1124.46783 Ha

F	-5.144452	0.826985	0.658691
C	-4.557512	0.162896	-0.351043
F	-5.261889	-0.969184	-0.517867
F	-4.714368	0.898757	-1.459951
C	-3.116394	-0.122087	-0.057909
C	-2.799123	-0.855263	1.088063
C	-1.478268	-1.135284	1.385040
C	-0.459014	-0.684596	0.536045
C	-0.770640	0.052519	-0.606384
C	-2.106167	0.327067	-0.895671
H	-2.355729	0.901604	-1.780775
H	0.006754	0.429679	-1.259120
O	0.803405	-1.033027	0.913607
C	1.901863	-0.641252	0.089039
C	2.161440	0.849388	0.132015
C	1.827689	1.603472	1.256730
C	2.113049	2.965562	1.292299
C	2.739093	3.578406	0.209416
C	3.077911	2.825564	-0.912916
C	2.787924	1.464611	-0.954432
H	3.049891	0.861591	-1.822040
H	3.563044	3.300169	-1.760394
H	2.959247	4.640992	0.238657
H	1.843157	3.550168	2.166393
H	1.332144	1.121578	2.094924
C	3.096667	-1.416746	0.621739
C	4.330975	-1.378307	-0.256738
N	3.960223	-1.722955	-1.628017
H	3.496056	-2.631931	-1.617663
H	5.089052	-2.040748	0.188308
H	4.748164	-0.362355	-0.251140
H	3.299705	-1.171642	1.669093
H	2.749242	-2.560844	0.615606
H	1.713807	-0.958133	-0.943266
H	-1.203196	-1.702024	2.268220
H	-3.591903	-1.203407	1.743445
O	2.093039	-3.640074	0.104036
H	1.203737	-3.297826	0.328308
H	4.793153	-1.816089	-2.203209

M1 site 7 OH

E=-1124.4684624 Ha

F	-5.112272	-0.950274	-0.759560
C	-4.498420	0.168938	-0.339731
F	-4.591317	1.062176	-1.335154
F	-5.217681	0.634929	0.693760
C	-3.075157	-0.089099	0.052093
C	-2.797822	-0.621653	1.312695
C	-1.492691	-0.910532	1.668242
C	-0.450385	-0.668376	0.764994

C	-0.721076	-0.129519	-0.496006
C	-2.040962	0.153284	-0.842014
H	-2.258323	0.578797	-1.815879
H	0.075995	0.083002	-1.198185
O	0.788351	-1.013765	1.210623
C	1.919514	-0.796065	0.394352
C	2.217720	0.666716	0.179106
C	1.842986	1.602313	1.146742
C	2.144494	2.949076	0.969321
C	2.816850	3.369876	-0.175555
C	3.187737	2.438449	-1.142967
C	2.888700	1.089664	-0.971729
H	3.179704	0.345591	-1.709396
H	3.707727	2.763699	-2.038911
H	3.047395	4.421601	-0.314888
H	1.850079	3.671132	1.724779
H	1.311782	1.270775	2.034404
C	3.042486	-1.609585	1.029219
C	4.367421	-1.542705	0.279011
N	4.168800	-1.831210	-1.138736
H	3.580297	-2.652551	-1.264623
H	5.070426	-2.224239	0.783309
H	4.783306	-0.531596	0.365399
H	3.179054	-1.254875	2.058208
H	2.693008	-2.647741	1.083360
H	1.717640	-1.300646	-0.646799
H	-1.247166	-1.325398	2.639742
H	-3.607138	-0.801996	2.012988
O	1.274347	-2.276620	-1.612825
H	0.358251	-2.388567	-1.286579
H	5.057847	-2.011610	-1.596203

M1 site 15 OH

E=-1124.4688064 Ha

F	5.297167	-1.237928	0.934172
C	4.781959	-0.164043	0.311097
F	5.017385	0.894730	1.100442
F	5.497250	0.002028	-0.813755
C	3.323345	-0.333967	0.017948
C	2.931129	-1.109922	-1.074823
C	1.587654	-1.317045	-1.328673
C	0.618361	-0.750178	-0.490952
C	1.006834	0.034095	0.597110
C	2.362971	0.232756	0.844767
H	2.670061	0.846201	1.685041
H	0.271874	0.507749	1.236037
O	-0.668796	-1.027563	-0.825106
C	-1.717818	-0.556613	0.015900
C	-1.914594	0.940873	-0.107886
C	-1.637744	1.593483	-1.309169
C	-1.858057	2.962877	-1.428893
C	-2.360493	3.688219	-0.351193
C	-2.639848	3.039642	0.849491
C	-2.414899	1.671023	0.972543
H	-2.634797	1.153147	1.903898
H	-3.027148	3.601393	1.694115
H	-2.529179	4.756468	-0.445175
H	-1.632523	3.465536	-2.364435
H	-1.234743	1.024688	-2.142481
C	-2.955581	-1.339224	-0.430102
C	-4.196945	-1.014702	0.384373
N	-3.987510	-1.240528	1.788687
H	-3.805782	-2.228746	1.956659
H	-5.037783	-1.701643	-0.014088
H	-4.531390	0.014955	0.220787
H	-3.139247	-1.122728	-1.489130
H	-2.733839	-2.410005	-0.345080
H	-1.495688	-0.813500	1.059468
H	1.254876	-1.916507	-2.169016
H	3.682947	-1.545183	-1.725690
O	-5.557366	-3.119792	-0.241122
H	-5.346050	-3.171869	-1.194070
H	-4.813571	-0.990537	2.325212

CH3OH_M1_N.out

M1 site 16 CH3OH

E=-1163.7636196 Ha

F	-5.054443	-0.357034	-1.714886
C	-4.864157	-0.455880	-0.390589
F	-5.486962	0.594167	0.172434
F	-5.513832	-1.553292	0.031246
C	-3.411012	-0.503320	-0.032739
C	-3.029157	-1.006087	1.212836
C	-1.695101	-1.010956	1.576557
C	-0.724821	-0.512651	0.697450
C	-1.103494	-0.006290	-0.547498
C	-2.450048	-0.007293	-0.903147
H	-2.749239	0.381913	-1.870494
H	-0.370390	0.400680	-1.232734
O	0.553452	-0.576308	1.152064
C	1.614500	-0.158690	0.298628
C	1.644214	1.347269	0.130149
C	1.240971	2.181065	1.173551
C	1.309787	3.564080	1.031800
C	1.786604	4.124067	-0.151244
C	2.191013	3.295470	-1.195134
C	2.116804	1.911759	-1.056542
H	2.432526	1.256971	-1.866374
H	2.557458	3.726507	-2.121875
H	1.837140	5.202845	-0.261404
H	0.985989	4.206353	1.845077
H	0.858025	1.738504	2.088935
C	2.880688	-0.691132	0.974463

C	4.156430	-0.350149	0.216135
N	4.073537	-0.807385	-1.160516
H	3.797472	-1.950533	-1.185027
H	5.024952	-0.768724	0.750531
H	4.307108	0.738932	0.189375
H	2.932241	-0.277287	1.987657
H	2.781295	-1.779580	1.055278
H	1.505977	-0.640023	-0.682064
H	-1.369118	-1.404201	2.533274
H	-3.780782	-1.401301	1.888933
O	3.847702	-3.152355	-0.907414
H	4.991697	-0.719960	-1.604875
C	4.909702	-3.480641	-0.074182
H	4.842796	-3.005098	0.917797
H	4.857831	-4.566047	0.088264
H	5.892637	-3.257256	-0.515978

M1 site 14 CH3OH

E=-1163.7624248 Ha

F	5.110309	1.336718	-0.314678
C	4.637526	0.274517	0.358985
F	5.420741	-0.765688	0.030155
F	4.824307	0.526144	1.663302
C	3.198956	0.004128	0.040802
C	2.872947	-0.699623	-1.120161
C	1.546346	-0.913215	-1.449158
C	0.530013	-0.422514	-0.619540
C	0.851780	0.286624	0.539906
C	2.191057	0.493363	0.861202
H	2.447938	1.041198	1.761624
H	0.077567	0.694546	1.178391
O	-0.735868	-0.701248	-1.026139
C	-1.816586	-0.409399	-0.144751
C	-2.160628	1.067887	-0.131611
C	-1.899588	1.868062	-1.243645
C	-2.251143	3.215262	-1.230831
C	-2.870382	3.766812	-0.111952
C	-3.136224	2.967345	0.998000
C	-2.781214	1.621405	0.991126
H	-2.988966	0.981731	1.846730
H	-3.615571	3.394538	1.873607
H	-3.142065	4.817815	-0.103291
H	-2.038058	3.836082	-2.095664
H	-1.408035	1.433456	-2.109197
C	-2.976946	-1.245112	-0.647475
C	-4.224609	-1.230163	0.207017
N	-3.866940	-1.535531	1.592188
H	-3.447496	-2.465883	1.606625
H	-4.953113	-1.927060	-0.235188
H	-4.675289	-0.228683	0.174783
H	-3.162470	-1.090074	-1.714503
H	-2.585229	-2.436978	-0.552801
H	-1.565449	-0.734207	0.872933
H	1.263920	-1.462620	-2.340991
H	3.662528	-1.087183	-1.756095
O	-2.257519	-3.559392	-0.055364
C	-0.861923	-3.556039	0.065467
H	-0.492577	-2.798378	0.772076
H	-0.598818	-4.543077	0.469387
H	-0.352138	-3.426740	-0.896900
H	-4.705490	-1.575243	2.165868

M1 site 7 CH3OH

E=-1163.7647964 Ha

F	-4.795549	1.454851	-0.096372
C	-4.490546	0.164129	-0.310630
F	-5.366128	-0.561071	0.403696
F	-4.725208	-0.080199	-1.608558
C	-3.074937	-0.147329	0.070221
C	-2.770798	-0.459348	1.394549
C	-1.456086	-0.694687	1.763330
C	-0.441239	-0.619004	0.806735
C	-0.738147	-0.312321	-0.522856
C	-2.061748	-0.078252	-0.880205
H	-2.305678	0.152045	-1.911887
H	0.042878	-0.279286	-1.273954
O	0.814999	-0.901692	1.267549
C	1.939761	-0.572658	0.491089
C	2.026338	0.891956	0.151401
C	1.514478	1.836511	1.046546
C	1.617117	3.194683	0.765133
C	2.226831	3.619228	-0.413158
C	2.734769	2.679904	-1.307358
C	2.635030	1.318920	-1.031597
H	3.042655	0.574091	-1.709249
H	3.207050	3.007121	-2.228597
H	2.302441	4.679391	-0.634634
H	1.217040	3.921708	1.465152
H	1.032255	1.501700	1.960889
C	3.139245	-1.164139	1.220935
C	4.485488	-0.884820	0.562763
N	4.459654	-1.238756	-0.852763
H	3.980421	-2.123164	-1.006402
H	5.252986	-1.418798	1.145035
H	4.709489	0.185920	0.644046
H	3.140036	-0.765804	2.243667
H	2.977082	-2.247401	1.299675
H	1.862164	-1.223899	-0.546191
H	-1.189097	-0.944095	2.784592
H	-3.564678	-0.523056	2.131542
O	1.737958	-2.222882	-1.421735
H	5.401956	-1.315590	-1.223633
C	0.905637	-3.178870	-0.836381
H	1.128191	-4.137829	-1.325488

H	1.117757	-3.307041	0.236478
H	-0.161368	-2.953771	-0.960210

M1 site 15 CH3OH

E=-1163.7659953 Ha

F	5.670315	-1.575258	0.138440
C	5.048571	-0.386929	0.216276
F	5.378823	0.166033	1.392885
F	5.584832	0.385874	-0.743824
C	3.566390	-0.529891	0.057559
C	3.065472	-1.400953	-0.912394
C	1.700433	-1.512547	-1.102306
C	0.818061	-0.753514	-0.322437
C	1.315410	0.121770	0.644962
C	2.692503	0.225145	0.827555
H	3.084137	0.901717	1.579535
H	0.649724	0.733222	1.241450
O	-0.500476	-0.952243	-0.582701
C	-1.471746	-0.288570	0.219748
C	-1.541576	1.194748	-0.081649
C	-1.247010	1.671648	-1.358839
C	-1.351840	3.031157	-1.639574
C	-1.755956	3.921976	-0.648052
C	-2.052677	3.449087	0.628153
C	-1.942873	2.090396	0.912034
H	-2.176592	1.709776	1.904287
H	-2.363529	4.139988	1.405939
H	-1.834624	4.982123	-0.867877
H	-1.113225	3.396388	-2.633758
H	-0.921397	0.973537	-2.124928
C	-2.790954	-1.002518	-0.094250
C	-3.962338	-0.478789	0.713379
N	-3.734912	-0.562682	2.124165
H	-3.585950	-1.528940	2.408555
H	-4.894043	-1.172524	0.417958
H	-4.239882	0.542513	0.434977
H	-2.998893	-0.892574	-1.164804
H	-2.655253	-2.073399	0.105206
H	-1.234775	-0.437601	1.281354
H	1.283593	-2.187631	-1.841736
H	3.749928	-1.995985	-1.508952
O	-5.696007	-2.290495	0.254798
C	-5.636360	-2.615891	-1.095795
H	-4.630450	-2.918380	-1.424799
H	-6.298431	-3.484130	-1.232856
H	-6.006738	-1.814029	-1.751093
H	-4.524134	-0.201196	2.651884

M2 site 6a CH3OH

E=-759.5187814 Ha

F	3.637153	0.806343	-0.452660
C	2.912000	-0.220859	0.016813
F	3.240226	-1.309138	-0.699124
F	3.334462	-0.450463	1.272723
C	1.442741	0.058659	-0.040795
C	0.972196	1.370816	-0.019873
C	-0.390829	1.623561	-0.018800
C	-1.295384	0.558127	-0.035821
C	-0.824499	-0.758843	-0.056990
C	0.541750	-1.002878	-0.058486
H	0.911455	-2.023152	-0.082287
H	-1.532966	-1.582972	-0.076546
O	-2.614410	0.850582	-0.034775
H	-0.779528	2.635864	-0.008434
H	1.677841	2.194941	-0.012195
H	-3.135184	0.024428	-0.047407
O	-4.620838	-1.090530	-0.032282
C	-5.613959	-0.142479	0.077516
H	-6.569075	-0.497506	-0.326200
H	-5.745174	0.005476	1.165737
H	-5.316044	0.825199	-0.346041

M2 site 6a CH3OH

E=-720.2020841 Ha

F	3.025814	0.968307	-0.159813
C	2.324130	-0.150430	0.071282
F	2.766092	-1.091580	-0.776407
F	2.641764	-0.564210	1.308436
C	0.848318	0.075419	-0.076225
C	0.311550	1.347362	0.114582
C	-1.059944	1.535953	0.043625
C	-1.897159	0.450721	-0.251575
C	-1.354089	-0.830601	-0.442188
C	0.014945	-1.011647	-0.346471
H	0.446463	-1.996672	-0.491627
H	-2.017286	-1.666148	-0.641575
O	-3.206591	0.697460	-0.388532
H	-1.509190	2.511656	0.191417
H	0.969220	2.184715	0.321597
H	-3.787040	-0.180149	-0.266534
O	-4.314848	-1.029380	0.605563
H	-4.960202	-0.511354	1.122350

Table S14. Cartesian Coordinates (in Å) and electronic energies (in Ha) for fluoxetine metabolites reactant complexes obtained with the HAT mechanism (radical ·OH and ·OCH_3). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

2 site 10 OH

E=-648.6639438 Ha

C	-2.257406	-0.951940	0.309797
C	-0.893695	-0.952817	0.071452
C	-0.251402	0.279589	-0.150525
C	-1.011598	1.468830	-0.141859
C	-2.388637	1.464392	0.098602
C	-3.000424	0.247299	0.327731
C	1.114095	0.648620	-0.438736
C	1.116158	2.013778	-0.593128
N	-0.148309	2.511490	-0.413583
C	2.286087	-0.255064	-0.505832
H	-0.331400	-1.883204	0.029778
H	-2.965331	2.384302	0.103807
H	-4.065596	0.182543	0.520276
H	1.946525	2.671482	-0.810201
H	-0.405794	3.483982	-0.468025
C	2.625393	-0.938628	0.815562
H	2.051968	-1.135173	-1.248775
H	3.167323	0.257259	-0.903988
N	3.064975	0.078680	1.767879
H	1.755494	-1.526442	1.148481
H	3.449155	-1.640262	0.651792
H	3.327146	-0.360507	2.647204
H	2.278834	0.693379	1.972701
O	-2.965968	-2.097647	0.535726
H	-2.358813	-2.850464	0.508435
O	1.355163	-2.255214	-1.818744
H	0.588837	-1.729538	-2.125818

M2 site 5a OH

E=-648.6658353 Ha

C	-2.122301	0.083000	0.410380
C	-0.916709	-0.498879	0.028469
C	0.176515	0.336700	-0.227042
C	0.032554	1.738186	-0.078794
C	-1.181547	2.324542	0.300940
C	-2.253660	1.487926	0.529975
C	1.534032	0.086203	-0.644969
C	2.140073	1.309633	-0.719180
N	1.245708	2.305520	-0.381903
C	2.159887	-1.254706	-0.879002
H	-0.848678	-1.576953	-0.091489
H	-1.281466	3.400604	0.404874
H	-3.221845	1.880884	0.819958
H	3.158062	1.551179	-0.992616
H	1.443254	3.293302	-0.389074
C	2.486745	-1.973493	0.434274
H	1.486042	-1.880364	-1.477005
H	3.090565	-1.135301	-1.443173
N	3.478399	-1.200378	1.177015
H	1.548622	-2.148739	0.988050
H	2.918082	-2.954066	0.206395
H	3.704776	-1.674420	2.047957
H	3.063914	-0.306299	1.435257
O	-3.212069	-0.652128	0.716076
H	-3.142927	-1.588664	0.325491
O	-3.406508	-2.362272	-0.880730
H	-4.372066	-2.316612	-1.013498

2 site 9 OH

E=-648.6641159 Ha

C	-2.307054	-1.247445	0.122752
C	-0.965050	-1.436032	-0.205132
C	-0.172285	-0.306134	-0.412548
C	-0.745774	0.976999	-0.327045
C	-2.081814	1.167645	0.015645
C	-2.857069	0.040262	0.241924
C	1.230889	-0.113766	-0.736947
C	1.418573	1.243239	-0.816163
N	0.227970	1.912275	-0.652953
C	2.253026	-1.188853	-0.920290
H	-0.553600	-2.439563	-0.296869
H	-2.489135	2.167489	0.122178
H	-3.902880	0.122863	0.515785
H	2.325825	1.785261	-1.047340
H	0.146176	2.944801	-0.308176
C	2.678141	-1.797290	0.423400
H	1.852333	-1.980841	-1.565199
H	3.143435	-0.777552	-1.405411
N	3.322181	-0.772361	1.237450
H	1.798335	-2.263673	0.898932
H	3.406509	-2.592736	0.234881
H	3.640502	-1.174153	2.115662
H	2.633812	-0.060823	1.476320
O	-3.154021	-2.290563	0.350252
H	-2.670677	-3.121669	0.244066
O	-0.035563	3.773172	0.793325
H	0.625487	3.518571	1.461504

2 site 11 OH

E=-648.66423 Ha

C	-2.474388	-1.298252	-0.011847
C	-1.134772	-1.103982	-0.295661
C	-0.626641	0.207205	-0.281427
C	-1.490550	1.282189	0.018917

C	-2.844519	1.082143	0.307643
C	-3.324289	-0.212345	0.290046
C	0.677341	0.763065	-0.532590
C	0.552411	2.118690	-0.372366
N	-0.742866	2.438997	-0.039919
C	1.927152	-0.000955	-0.850536
H	-0.490201	-1.948609	-0.531962
H	-3.503158	1.914204	0.537266
H	-4.365255	-0.427680	0.504452
H	1.300810	2.891499	-0.486455
H	-1.097362	3.371910	0.095851
C	2.454377	-0.777557	0.350307
H	1.751181	-0.702235	-1.673996
H	2.717321	0.683614	-1.177957
N	2.850102	0.105976	1.416246
H	1.783384	-1.596728	0.649513
H	3.440152	-1.311644	-0.031493
H	2.884825	-0.374831	2.309597
H	2.185658	0.874249	1.498552
O	-3.059273	-2.533705	-0.003164
H	-2.395493	-3.196221	-0.239580
O	4.789686	-1.205398	-0.377671
H	4.897455	-0.440729	0.223696

2 site 12 OH

E=-648.6650446 Ha

C	2.339531	-1.251783	0.164493
C	1.101946	-0.910346	0.679054
C	0.578196	0.362029	0.386657
C	1.325243	1.250219	-0.417376
C	2.576792	0.901664	-0.935762
C	3.072792	-0.352150	-0.638995
C	-0.641074	1.036374	0.750185
C	-0.585894	2.271202	0.158674
N	0.588692	2.408778	-0.542627
C	-1.766641	0.468332	1.560131
H	0.548424	-1.611339	1.301030
H	3.145738	1.590938	-1.552280
H	4.037269	-0.677040	-1.013347
H	-1.307474	3.076275	0.192210
H	0.878164	3.234818	-1.040902
C	-2.554444	-0.598299	0.785137
H	-1.379056	0.014746	2.480769
H	-2.454089	1.267779	1.855865
N	-3.167288	0.007570	-0.386955
H	-1.883266	-1.426334	0.516080
H	-3.352079	-1.009198	1.410267
H	-3.771458	-0.714227	-0.944456
H	-2.432219	0.378719	-0.993029
O	2.929364	-2.463388	0.393482
H	2.345052	-2.996193	0.950342
O	-3.681811	-1.947269	-1.565377
H	-2.983924	-1.821576	-2.233504

2 site 10 CH3OH

E=-687.9574113 Ha

C	2.108297	1.491001	0.368757
C	0.814705	1.028338	0.202006
C	0.630355	-0.316886	-0.155950
C	1.752473	-1.144568	-0.365131
C	3.057432	-0.675100	-0.191620
C	3.221788	0.644290	0.184693
C	-0.543576	-1.109824	-0.430615
C	-0.086802	-2.352258	-0.806393
N	1.281998	-2.382687	-0.761070
C	-1.945860	-0.688619	-0.269336
H	-0.042173	1.693191	0.288412
H	3.917814	-1.317566	-0.352326
H	4.210224	1.065907	0.330577
H	-0.653549	-3.229762	-1.085430
H	1.854878	-3.180569	-0.985153
C	-2.353268	-0.375469	1.165423
H	-2.053578	0.377167	-0.865425
H	-2.649611	-1.388599	-0.729503
N	-2.294226	-1.608582	1.947839
H	-1.715986	0.437745	1.550026
H	-3.387841	-0.015187	1.178268
H	-2.567433	-1.421879	2.909963
H	-1.326651	-1.926269	1.975157
O	2.389497	2.784198	0.710868
H	1.558481	3.276488	0.764485
O	-2.143754	1.659367	-1.205358
C	-3.432103	2.064229	-0.862649
H	-3.581953	2.168522	0.222183
H	-3.573682	3.056499	-1.315225
H	-4.209926	1.403873	-1.272577

2 site 5a CH3OH

E=-687.9686668 Ha

C	1.828280	0.419547	-0.783582
C	0.711939	-0.314818	-0.354033
C	-0.399921	0.375440	0.134374
C	-0.378851	1.792555	0.169970
C	0.736199	2.535186	-0.250695
C	1.833807	1.840994	-0.706131
C	-1.676981	-0.048878	0.655517
C	-2.358930	1.094736	0.963490
N	-1.583632	2.202382	0.676422
C	-2.170064	-1.459393	0.761487
H	0.743996	-1.400388	-0.397940
H	0.737802	3.620133	-0.209605
H	2.729542	2.354027	-1.038044
H	-3.353488	1.208308	1.372160

H	-1.855022	3.159840	0.835450
C	-2.613358	-2.016219	-0.595873
H	-1.380900	-2.098839	1.175667
H	-3.025273	-1.501705	1.443488
N	-3.740777	-1.234787	-1.096314
H	-1.744367	-2.036804	-1.275226
H	-2.946801	-3.050746	-0.463139
H	-4.063692	-1.620982	-1.980047
H	-3.418887	-0.289300	-1.296124
O	2.904815	-0.177412	-1.290251
H	3.064029	-1.096856	-0.799938
O	3.357152	-1.957162	0.212773
C	3.207594	-1.414061	1.460149
H	4.160835	-1.242988	1.978536
H	2.570702	-2.071259	2.078349
H	2.638373	-0.459539	1.407432

2 site 11 CH3OH

E=-687.9609796 Ha

C	-2.807194	-1.359186	-0.019948
C	-1.471398	-1.112050	-0.279601
C	-1.019365	0.219458	-0.273588
C	-1.933661	1.260902	-0.005905
C	-3.283588	1.007424	0.258804
C	-3.707914	-0.306399	0.249971
C	0.265309	0.826117	-0.505581
C	0.080122	2.177178	-0.367533
N	-1.234391	2.447534	-0.065896
C	1.553693	0.112207	-0.784024
H	-0.787172	-1.931302	-0.492180
H	-3.981251	1.813747	0.463684
H	-4.743108	-0.562661	0.446593
H	0.796859	2.979797	-0.480076
H	-1.630644	3.366290	0.048895
C	2.071598	-0.666383	0.419817
H	1.443783	-0.582120	-1.624231
H	2.324690	0.836222	-1.075267
N	2.341772	0.178157	1.530165
H	1.469939	-1.554857	0.656042
H	3.130774	-1.129622	0.021422
H	2.292933	-0.288798	2.427474
H	1.762399	1.014590	1.536919
O	-3.339609	-2.618173	-0.006133
H	-2.643856	-3.254591	-0.221439
O	4.329876	-1.257484	-0.539309
C	5.087980	-0.214640	-0.025144
H	4.494753	0.359284	0.713503
H	5.976634	-0.593095	0.501920
H	5.405973	0.484768	-0.813211

2 site 12 CH3OH

E=-687.9595263 Ha

C	2.309235	-1.149777	0.508471
C	1.128786	-0.603651	0.979723
C	0.664315	0.595237	0.406850
C	1.414352	1.206049	-0.621273
C	2.608744	0.651976	-1.093890
C	3.044796	-0.526627	-0.522960
C	-0.489507	1.424242	0.644219
C	-0.393567	2.472908	-0.233556
N	0.745053	2.352206	-0.993224
C	-1.601558	1.146147	1.608624
H	0.575843	-1.090413	1.780947
H	3.179433	1.129017	-1.884802
H	3.962638	-1.002673	-0.849736
H	-1.061148	3.313333	-0.368266
H	1.048671	3.004062	-1.698520
C	-2.435486	-0.073012	1.180499
H	-1.199928	0.956877	2.611650
H	-2.258899	2.019193	1.684440
N	-3.088594	0.170860	-0.093769
H	-1.771518	-0.950980	1.118656
H	-3.202075	-0.296140	1.928885
H	-3.367345	-0.856984	-0.582826
H	-2.383367	0.579779	-0.719140
O	2.838402	-2.309117	1.000884
H	2.255917	-2.651521	1.692986
O	-3.053080	-2.000478	-0.954679
C	-1.801572	-2.009803	-1.565890
H	-0.988271	-1.715314	-0.880974
H	-1.604728	-3.046086	-1.872767
H	-1.754244	-1.378991	-2.466128

2 site 9 CH3OH

E=-687.9619001 Ha

C	-2.673747	-0.716372	0.283171
C	-1.454464	-1.305306	-0.065154
C	-0.433832	-0.475663	-0.519811
C	-0.655974	0.907388	-0.664317
C	-1.863501	1.495085	-0.299609
C	-2.871901	0.668726	0.179161
C	0.946633	-0.710401	-0.924876
C	1.447898	0.518239	-1.271685
N	0.485353	1.503463	-1.197700
C	1.665089	-2.018891	-0.896073
H	-1.314700	-2.381167	0.023601
H	-2.004032	2.568166	-0.377106
H	-3.833350	1.069481	0.479742
H	2.446978	0.758631	-1.611973
H	0.784159	2.489576	-0.710778
C	2.067985	-2.392950	0.538684
H	1.028806	-2.809555	-1.312362
H	2.574194	-1.960260	-1.501843
N	3.010785	-1.404948	1.049886

H	1.154121	-2.503995	1.147352
H	2.567906	-3.366809	0.519843
H	3.311574	-1.660525	1.986933
H	2.539754	-0.505082	1.128743
O	-3.724503	-1.447810	0.744930
H	-3.475671	-2.382186	0.774129
O	1.031298	3.162269	0.384588
C	1.540963	2.346529	1.375063
H	1.497351	2.898316	2.326452
H	0.919496	1.439919	1.518636
H	2.585183	2.041907	1.199858

2 site 5a OOH

E=-723.8128943 Ha

C	-1.828324	0.858736	0.461163
C	-0.799858	-0.037079	0.086870
C	0.457934	0.479806	-0.218836
C	0.681952	1.876747	-0.125480
C	-0.330913	2.779042	0.255831
C	-1.572593	2.264457	0.530182
C	1.701319	-0.126935	-0.636467
C	2.597740	0.895349	-0.764541
N	1.987270	2.100303	-0.459403
C	1.956166	-1.590944	-0.821923
H	-1.011896	-1.100856	0.047679
H	-0.136397	3.845288	0.321471
H	-2.400729	2.903226	0.816178
H	3.638484	0.862628	-1.055121
H	2.433019	3.003710	-0.498426
C	2.129893	-2.316173	0.517158
H	1.124795	-2.043925	-1.375030
H	2.868257	-1.735585	-1.409619
N	3.305337	-1.790223	1.206317
H	1.194254	-2.229931	1.094784
H	2.295515	-3.381143	0.323778
H	3.445923	-2.291227	2.080217
H	3.128439	-0.819058	1.457525
O	-3.032271	0.421881	0.759091
H	-3.237602	-0.407801	0.055385
O	-3.312335	-1.274125	-0.887983
O	-3.206569	-2.435325	-0.157573
H	-3.940815	-2.973370	-0.499250

2 site 5a OOCH3

E=-763.1086045 Ha

C	-1.100688	1.510533	0.479433
C	-0.406816	0.336232	0.107374
C	0.943578	0.433093	-0.221922
C	1.591493	1.693099	-0.155583
C	0.914505	2.869788	0.220614
C	-0.421076	2.768785	0.518333
C	1.930468	-0.534514	-0.644829
C	3.097074	0.157465	-0.801859
N	2.895908	1.496300	-0.509972
C	1.716028	-2.007727	-0.807065
H	-0.941533	-0.608312	0.083404
H	1.430615	3.824105	0.264597
H	-1.005547	3.636603	0.802922
H	4.071212	-0.200208	-1.104885
H	3.598794	2.216350	-0.571142
C	1.675971	-2.732544	0.542865
H	0.777129	-2.188076	-1.343965
H	2.529554	-2.436246	-1.401055
N	2.966612	-2.587886	1.211212
H	0.822003	-2.351835	1.127952
H	1.500052	-3.798914	0.366943
H	2.956252	-3.092617	2.094176
H	3.104276	-1.605774	1.443797
O	-2.373527	1.471156	0.805430
H	-2.855410	0.738112	0.114859
O	-3.248363	-0.073090	-0.778098
O	-3.461199	-1.186844	-0.012135
C	-4.781424	-1.642224	-0.242911
H	-5.501337	-0.879078	0.067999
H	-4.918634	-1.870516	-1.303873
H	-4.895031	-2.544188	0.361310

2 site 5a OOCHCH2

E=-801.1906352 Ha

C	0.610922	-1.707363	0.504227
C	0.071236	-0.452914	0.132027
C	-1.269869	-0.387957	-0.239141
C	-2.063627	-1.562787	-0.211129
C	-1.541632	-2.815014	0.170715
C	-0.214831	-2.875650	0.512320
C	-2.122479	0.695025	-0.675139
C	-3.357139	0.147652	-0.876774
N	-3.323571	-1.209111	-0.599932
C	-1.730270	2.133935	-0.809045
H	0.711077	0.423025	0.139317
H	-2.167266	-3.702318	0.186098
H	0.254196	-3.808970	0.802833
H	-4.272735	0.621197	-1.202357
H	-4.105286	-1.839560	-0.689302
C	-1.646108	2.832815	0.552606
H	-0.760867	2.207709	-1.316101
H	-2.469041	2.662943	-1.419335
N	-2.964624	2.834764	1.180586
H	-0.861334	2.346804	1.156410
H	-1.339924	3.872594	0.397872
H	-2.924107	3.330991	2.067454
H	-3.223149	1.874389	1.400394

O	1.868784	-1.833309	0.863726
H	2.439106	-1.087385	0.315765
O	2.970411	-0.199815	-0.513075
O	3.374902	0.749107	0.385404
C	5.421084	0.855806	-0.868669
H	5.119595	0.090845	-1.570765
H	6.391686	1.323604	-0.968782
H	4.860078	1.992291	0.859934
C	4.618140	1.233855	0.122592

Table S15. Cartesian Coordinates (in Å) and electronic energies (in Ha) for isolated radicals. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

CH3OOH
E=-190.8293897 Ha

O	-1.147069	0.270796	0.102545
O	-0.025279	-0.605400	0.019773
H	-1.569086	0.104132	-0.756207
C	1.115476	0.222340	-0.021549
H	1.963984	-0.466065	-0.031970
H	1.125724	0.842163	-0.925757
H	1.165302	0.862565	0.864682

CH3OO
E=-190.1880031 Ha

O	1.169320	-0.278307	0.000017
O	0.157975	0.542855	-0.000016
C	-1.081506	-0.181434	-0.000021
H	-1.130743	-0.801366	-0.896590
H	-1.131372	-0.800256	0.897305
H	-1.867213	0.573839	-0.000590

HOH
E=-76.4207431 Ha

O	0.000000	0.000000	0.118437
H	-0.000000	0.762918	-0.473747
H	-0.000000	-0.762918	-0.473747

HO
E=-75.726486 Ha

O	-0.000000	-0.000000	0.108762
H	0.000000	0.000000	-0.870096

CH2CHOOH
E=-228.9100758 Ha

C	1.406517	-0.554260	0.001289
C	0.696641	0.565615	0.013829
H	0.940238	-1.527673	-0.060358
H	2.485961	-0.488479	0.033521
H	1.124964	1.562825	0.054755
O	-0.663060	0.702224	-0.016204
O	-1.287489	-0.566962	-0.101344
H	-1.565717	-0.696899	0.821765

CH2CHOO
E=-228.2642065 Ha

C	-1.389731	-0.500063	0.000186
C	-0.628608	0.583193	-0.000384
H	-0.954065	-1.490586	0.001155
H	-2.466422	-0.390841	-0.000307
H	-0.972696	1.610046	-0.001325
O	0.762674	0.580046	0.000699
O	1.300227	-0.608472	-0.000491

CH3OH
E=-115.7041388 Ha

C	-0.046785	0.658091	-0.000000
H	-1.091646	0.973590	-0.000000
H	0.437523	1.077763	0.891937
H	0.437523	1.077763	-0.891937
O	-0.046785	-0.753213	0.000000
H	0.871595	-1.051960	0.000000

CH3O
E=-115.0303887 Ha

C	-0.009738	-0.577810	0.000000
H	1.056999	-0.867510	0.000000
H	-0.460335	-1.006509	0.905992
H	-0.460335	-1.006509	-0.905992
O	-0.009738	0.793424	-0.000000

HOOH
E=-151.5350859 Ha

O	0.000000	0.713705	-0.055572
O	-0.000000	-0.713705	-0.055572
H	-0.812252	-0.891397	0.444578
H	0.812252	0.891397	0.444578

HOO
E=-150.8904372 Ha

O	0.055503	0.709875	-0.000000
O	0.055503	-0.601901	0.000000
H	-0.888054	-0.863793	0.000000